

On Some Rigidity Properties in PDEs

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Introduction

This thesis is dedicated to two types of “rigidity properties” occurring in certain PDEs. These rigidity notions are rather complementary – the first originating from the study of controllability, the second appearing in the context of material sciences. While the first notion of rigidity is typical of elliptic (and parabolic) equations, the second one is mainly associated with hyperbolic equations and systems.

Before describing precisely the setting of our problems, we recall two prototypes of the rigidity properties we have in mind:

- The first rigidity property we deal with is associated with the unique continuation principle. Here the model operator is given by the Laplacian. Due to its analyticity, a solution which vanishes of infinite order at a point must already vanish globally.

Thus, a naturally arising question is whether this extends to more general operators and, in the case of a positive answer, to which ones. In this thesis we deal with two problems of such a flavour: The first is concerned with a parabolic “unique continuation problem at infinity”, while the second treats the unique continuation problem for the fractional Laplacian. In the second problem we put a particular emphasis on requiring as little regularity as possible.

- The second rigidity problem we investigate concerns a system of PDEs and is related to the notion of characteristics (in first order equations). Although we are confronted with a system, this type of “rigidity property” is already present in scalar (hyperbolic) equations: A toy problem would, for example, be the transport equation for which the characteristics of the system are straight lines. A more elaborate (toy) model is, for instance, given by the following two-dimensional gradient inclusion problem:

$$\nabla u \in \left\{ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \right\} + Skew(2).$$

Using the discreteness of the symmetrized gradient and the compatibility conditions, one finds that solutions, u , either satisfy $e(\nabla u) := \frac{1}{2}(\nabla u + (\nabla u)^t) = f(x_1 - x_2)$ or $e(\nabla u) = g(x_1 + x_2)$. Thus in both examples, the scalar transport

equation and the differential inclusion, the solutions are necessarily of the form of waves propagating along certain characteristics. In this sense the solutions are very rigid. We remark that although solving a PDE with the method of characteristics is not uncommon when dealing with *scalar* equations, it often poses problems in the context of *systems* as the resulting equations are not closed.

In this thesis we deal with the classification of all possible solutions of a certain (vector-valued) differential inclusion which arises in the study of phase transitions in certain shape-memory materials such as CuAlNi. For this transition we prove two complementary results: On the one hand, one cannot hope for rigidity for a too weak notion of a solution. On the other hand, adding regularity constraints, the problem becomes rigid and only very specific, essentially two-dimensional patterns occur.

Keeping this brief description of the different notions of rigidity in mind, we present the problems which are discussed in this thesis in greater detail:

The backward uniqueness property in conical domains. This problem deals with the controllability of the heat equation (and perturbations thereof):

$$\begin{aligned}\partial_t u - \Delta u &= W_1 u + W_2 \cdot \nabla u \text{ in } \Omega_\theta \times (0, T), \\ u &= u_0 \text{ in } \Omega_\theta \times \{0\},\end{aligned}$$

Here Ω_θ is a cone with opening angle θ .

We aim at understanding the interplay of the strong diffusivity and the unbounded underlying geometry. As is known since, for example, the work of Zuazua and Micu [MZ01a], [MZ01b], there is a major discrepancy between bounded and unbounded domains. While the heat equation is null-controllable, i.e. by choosing adapted boundary data it is possible to drive any L^2 (initial) datum to zero in an arbitrarily short time interval, in *bounded* domains, this is no longer the case in *unbounded* domains. On top of that depending on the “degree of unboundedness of the domain”, the heat equation is not only not null-controllable but even displays the backward uniqueness property, i.e. in conical domains with sufficiently large opening angles the only solution which can be driven to zero is the trivial solution.

In the first part of the thesis we provide a quantitative description of the large angle regime in two spatial dimensions. In this context, it is known that the backward uniqueness property can only hold in angles larger than 90° which is a consequence of the Phragmen-Lindelöf principle [ESŠ03], [SŠ02]. Furthermore, it is conjectured that the backward uniqueness property actually holds in all angles larger than 90° , reflecting the fact that the diffusivity is not strong enough to drive any nontrivial L^2 datum to zero. However, the furthest previous result in this direction only shows that the backward uniqueness property holds in all angles down to approximately 109° [LŠ10].

Motivated by understanding a related *elliptic* “unique continuation problem at infinity”, we aim at improving this bound in two spatial dimensions via a more detailed phase space analysis. As in the paper by Šverák and Li [LŠ10], the core of our approach relies on Carleman estimates, i.e. exponentially weighted estimates of the type

$$\|e^{\tau\phi}u\|_{L^2} \lesssim \|e^{\tau\phi}(\partial_t + \Delta)u\|_{L^2}, \quad \tau \geq \tau_0.$$

Here, the main novelty in dealing with the backward uniqueness problem is the identification of a necessary pseudoconvexity condition for a large class of two-dimensional weight functions. Working with a product ansatz for the Carleman weight, we obtain an ordinary differential inequality on the characteristic set. Using solutions of this, we can prove the backward uniqueness property in conical domains with opening angles down to approximately 95° in two dimensions.

The unique continuation property for fractional Schrödinger operators.

The unique continuation problem for Schrödinger operators is by now well-understood, c.f. [JK85], [KT01a]. Motivated by dealing, for example, with the absence of positive eigenvalues, c.f. [KT06], [IJ03], the main task was to understand up to which “degree of roughness” of the potentials and metrics, the unique continuation principle persists. Here, the threshold is provided by the respective scaling-critical L^p and Lorentz spaces.

Thinking about unique continuation, an interesting question concerns the interplay of the *local* property of infinite order vanishing and *non-local* operators: How strongly does the local property interact with non-local operators such as the fractional Laplacian? Does the fractional Laplacian mirror the behaviour of its “local relative”, the Laplacian? More precisely, does

$$(-\Delta)^s u = Vu \text{ in } \mathbb{R}^n,$$

with $u \in H_{loc}^s(\mathbb{R}^n)$, $s \in (0, 1)$, $\lim_{r \rightarrow 0} r^{-m} \int_{B_r(0)} u^2 dx = 0$ for all $m \in \mathbb{N}$ and V being in an appropriate class of potentials, already imply $u \equiv 0$?

In the chapter dedicated to the unique continuation properties of the fractional Laplacian we deal with these questions via Carleman inequalities and thus complement and extend results from the literature.

Here, the furthest previous results concerning unique continuation properties of the fractional Laplacian are in the article [FF13] by Fall and Felli. The authors approach the unique continuation property for the fractional Laplacian via frequency function methods. They prove that for $C^1(\mathbb{R}^n \setminus \{0\})$ perturbations of certain scaling-critical Hardy potentials the strong unique continuation property holds. We extend and complement these results in several aspects, of which two of the most important are:

- “*Rough*” potentials. It is possible to weaken various assumptions: If $s \in [\frac{1}{2}, 1)$

we, for example, prove the strong unique continuation property for potentials $V(y) = |y|^{-2s} f(\frac{y}{|y|}) + V_2(y)$, $|V_2(y)| \lesssim |y|^{-2s+\epsilon}$ which, in particular, include scaling-critical potentials. However, these need neither be of Hardy type nor small. Moreover, in one-dimensional settings and if $s \geq \frac{1}{2}$ we show an analogue of a result of Pan [Pan92] by proving the strong unique continuation property for $|V(y)| \leq c|y|^{-2s}$.

- *Flexibility.* Our Carleman methods carry over to more general settings of unique continuation at the boundary of a domain. In particular, it is possible to treat perturbations of the metrics under consideration. Hence, we can deal with “variable coefficient” fractional Schrödinger operators.

In dealing with the unique continuation principle, we argue via a combination of Carleman estimates and a blow-up analysis. In particular, the Carleman estimates imply doubling inequalities from which we obtain compactness. These allow to reduce the *strong* unique continuation problem to the *weak* unique continuation problem.

As already pointed out, the second part of the thesis is dedicated to capturing a different rigidity property. Motivated by pictures of experimental configurations of the cubic-to-orthorhombic phase transition, we investigate this phase transition which occurs in certain shape-memory alloys. Here we proceed in two steps:

Non-rigidity properties of the cubic-to-orthorhombic phase transition. As a first step we prove that sufficiently weak solutions ($u \in W^{1,p}(\Omega)$, $p \in (1, \infty)$) of the partial differential inclusion associated with the so-called cubic-to-orthorhombic phase transition, i.e.

$$e(\nabla u) = \frac{\nabla u + (\nabla u)^t}{2} \in \{e^{(1)}, \dots, e^{(6)}\}, \quad (0.0.1)$$

$$e^{(1)} = \epsilon \begin{pmatrix} 1 & \delta & 0 \\ \delta & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}, \quad e^{(2)} = \epsilon \begin{pmatrix} 1 & -\delta & 0 \\ -\delta & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}, \quad e^{(3)} = \epsilon \begin{pmatrix} 1 & 0 & \delta \\ 0 & -2 & 0 \\ \delta & 0 & 1 \end{pmatrix},$$

$$e^{(4)} = \epsilon \begin{pmatrix} 1 & 0 & -\delta \\ 0 & -2 & 0 \\ -\delta & 0 & 1 \end{pmatrix}, \quad e^{(5)} = \epsilon \begin{pmatrix} -2 & 0 & 0 \\ 0 & 1 & \delta \\ 0 & \delta & 1 \end{pmatrix}, \quad e^{(6)} = \epsilon \begin{pmatrix} -2 & 0 & 0 \\ 0 & 1 & -\delta \\ 0 & -\delta & 1 \end{pmatrix},$$

are not rigid. We illustrate that, on the contrary, a very large set of boundary values can be accommodated without causing stresses (e.g. for affine boundary data Mx we only require $e(M) \in \text{intconv}(e^{(1)}, \dots, e^{(6)})$).

Using the framework of convex integration as developed by Müller and Šverák [MŠ99], we construct a sequence of functions which comes closer and closer to being a solution of the differential inclusion by successively adding increasingly high oscillations. Working in the framework of the linear theory of elasticity, the differential

inclusion involves an unbounded component. Thus, in order to obtain sufficient compactness properties for the sequence of “almost solutions” to yield a solution in the limit an additional tool is needed. This is provided by Korn’s inequality.

Non-rigidity phenomena in models describing shape-memory alloys as such are not new: In the framework of *nonlinear* elasticity already the simplest toy model, the two-well problem, displays non-rigidity for weak solutions. A similar behaviour is known for the cubic-to-tetragonal phase transition: Again, in the nonlinear theory, weak solutions are not rigid. However, for all these examples the *linear* theory of elasticity differs dramatically: For the linearized versions of the discussed problems, there are very strong rigidity properties. In this sense, the cubic-to-orthorhombic phase transition can be considered as one of the simplest (real-life) transitions in which this lack of rigidity can already occur in the framework of the linear theory of elasticity. This is due to the presence of “sufficiently many” different phases.

Rigidity properties of the cubic-to-orthorhombic phase transition. Introducing regularity constraints (i.e. surface energy), we prove a rigidity result for solutions of the cubic-to-orthorhombic phase transition. If the solutions are piecewise affine, i.e. the support of the different phases consists of an arbitrary but finite number of polygonal domains, then the solutions are locally very rigid for generic parameters of δ : Formulated in the whole space setting, we prove the following proposition (c.f. Chapter 6 for the notation):

Proposition 1. *Let $\delta \notin \{\pm\frac{3}{2}, \pm 3\}$. Then, any configuration such that the support of each phase consists a union of only finitely many different polygons (also infinitely extended polygons are allowed) and which satisfies (0.0.1) in \mathbb{R}^n is either a twin or a crossing-twin pattern.*

This phenomenon of complementing a non-rigidity result has been observed both in the nonlinear two-well problem and the nonlinear cubic-to-tetragonal phase transition. However, both of these differential inclusions exhibit much clearer structures than our problem: Whereas the first can be reduced to its linearized version (for which one has rigidity) if the solutions are in BV, the second one is “sufficiently small” to handle its rank-one connections combinatorially. As our model contains 21 different symmetrized rank-one connections and as it displays non-rigidity already in the linearized setting, none of these strategies can be applied.

Instead, we argue via a classification of zero-homogeneous configurations which are obtained by a mixture of combinatorial and analytical arguments. In a second step these local constructions are used in order to deduce a characterization of global solutions. Again, this involves strong combinatorial elements.

Part I

**Rigidity Properties in
Inverse Problems and Unique
Continuation**

Chapter 1

Introduction

In this first part of the thesis we are concerned with two “rigidity properties” originating from the field of “inverse problems”. In general, these are problems in which certain data are given or measured from which one tries to reconstruct certain unknown parameters of the model.¹ A typical problem from applications would, for example, be to measure currents at the boundary of a material and deduce properties (inclusions, fractions, conductivities etc.) of the given sample. This allows to use non-invasive strategies in the investigation of materials but also in medicine (e.g. tomography).

Mathematically, problems from this field are “inverses” to the “usual” questions in the sense that one “reverses” the dependences with respect to the “usual” treatment of an equation. Instead of starting from initial and boundary data, u_0 , u_1 , from some space X , and asking how this influences the equation (e.g. in terms of well-posedness), one begins with a (well-posed) equation from which one would like to recover certain information (e.g. boundary data, initial data, conductivities), c.f. [Isa06].

In the sequel we will be confronted with such a problem in treating backward uniqueness properties of the heat equation. Here, we pose the question whether for given initial data it is possible to find boundary data such that in certain conical domains with sufficiently large opening angles the solution of the heat equation with these data is driven to zero at the final time (this is the so-called null-controllability problem). In this context a typical feature of inverse problems is displayed: Whereas the original problem, i.e. in our case the heat equation, is a well-posed and well-understood problem, the inverse question turns out to be highly ill-posed. This

¹The term “inverse problem” is not defined very precisely; in the sequel we refer to it in the sense of Isakov, [Isa06]: “An inverse problem assumes a direct problem that is a well-posed problem of mathematical physics. In other words, if we know completely a “physical device”, we have a classical mathematical description of this device including uniqueness, stability, and existence of a solution of the corresponding mathematical problem. But if one of the (functional) parameters describing this device is to be found from (additional boundary/experimental) data, then we arrive at an inverse problem.”

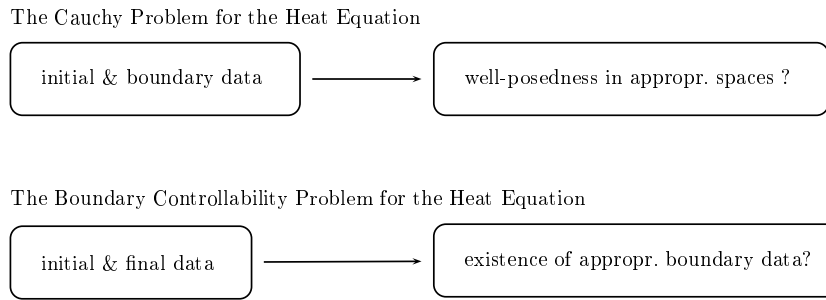


Figure 1.1: A schematic comparison of the Cauchy and the boundary controllability problem for the heat equation. While the first is well-posed in the standard spaces, the inverse problem is highly ill-posed.

ill-posedness is reflected in the fact that, in general, there are no solutions (in L^2) of the backward heat equation with zero final data and given initial data in L^2 in conical domains with sufficiently large opening angles.

This can be interpreted as a rigidity result for solutions of the heat equation in “sufficiently unbounded” domains: Via L^2 initial and boundary data it is not possible to introduce sufficiently high oscillations into the evolution of the heat equation so as to create strong cancellations.

The second problem treated in this first part of the thesis can also be regarded as a rigidity property. In studying the fractional Laplacian, it is natural to ask whether (and to which extent) it shares the strong rigidity properties of its local “relative” – the Laplacian. Thus, we discuss the (strong) unique continuation problem for the fractional Laplacian. This corresponds to the following uniqueness question: If a solution to an appropriate fractional Schrödinger equation vanishes of infinite order at a given point, does this already imply that it vanishes globally? As this property holds true for (local) Schrödinger equations with appropriately chosen potentials, it seems plausible that this property is shared by its non-local analogue. However, a key challenge consists of relating the local information of infinite order vanishing and the non-locality of the operator. As in the first problem, mathematically, the main task is the derivation of appropriate *lower bounds* – i.e. ruling out (too strong) oscillations.

Proving these *lower bounds* requires strong techniques which can, for instance, deal with possible oscillations and which utilize the given local information (boundary data, infinite order of vanishing) in a highly efficient manner. For that purpose we rely on a relatively abstract approach first introduced by Carleman [Car39] in the context of uniqueness issues of certain Cauchy problems. As this constitutes the central mathematical tool in our analysis of both problems, we briefly point out its key ideas.

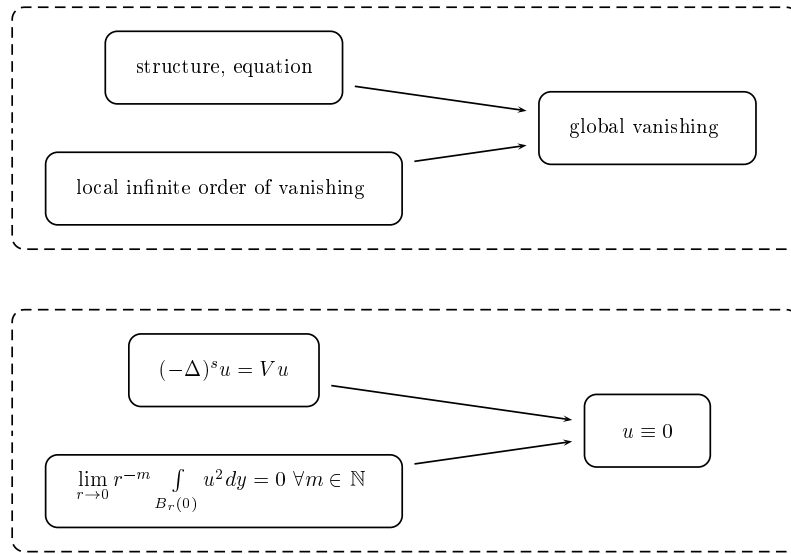


Figure 1.2: The (strong) unique continuation problem: In the upper box a general unique continuation principle is illustrated schematically. In the lower box this is applied to the unique continuation problem for the fractional Laplacian. We aim at finding appropriate conditions on V which ensure the strong unique continuation property.

The Backward Uniqueness Property, Unique Continuation and Carleman Estimates

Both properties which we seek to understand in this part of the thesis can be phrased in a broader common framework. In both cases we aim at characterizing solutions of certain equations by making use of their structure (which is determined by the equation which they satisfy). Additionally, very specific information is given at certain parts of the domain: In the unique continuation setting this information is evidently the vanishing of infinite order at a given point. In the investigation of the backward uniqueness property the information appears to be of a different type. At first sight it seems to be restricted to the knowledge of the initial and final state. However, it encodes more. In a sense, it is possible to interpret the backward uniqueness property as a unique continuation property at infinity: The null-controllability condition implies Gaussian decay at infinity. From this point of view, both problems are closely related, which also explains the similarity in the tools which we use to approach them.

The techniques, which we employ in dealing with the problems, originate from the field of unique continuation. Thus, these are designed to replace more delicate tools such as power series expansions or Holmgren's theorem. One of the key methods are so-called Carleman estimates. These are inequalities using weights of extremely high concentration in certain parts of the underlying domain. As a consequence, they are very popular and successful tools in proving unique continuation results,

for which one can create concentration close to the points at which information on the function under consideration is given (e.g. close to a zero of infinite order), c.f. for example the articles [JK85], [KRS87], [KT01b], [CK10], [KT09], [Ken89], [Wol93], [KT01a], [Tat96], [Tat99b]. In their simplest form, Carleman estimates are inequalities of the following type

$$\left\| e^{\phi(x,\tau)} u \right\|_{L^2(\Omega)}^2 \lesssim \left\| e^{\phi(x,\tau)} P(x, D) u \right\|_{L^2(\Omega)}^2 \quad \text{for all } \tau \geq \tau_0, \quad (1.0.1)$$

for all $u \in C_0^\infty(\Omega)$. Here, in its easiest form, $\phi(x, \tau)$ can be thought of as $\tau\psi(x)$, and $P(x, D)$ represents an operator which is controlled in the desired applications. Thus, up to an error term, the right hand side of the inequality is very small, while the left hand side explodes as $\tau \rightarrow \infty$.

At first sight such an inequality might appear to be a standard estimate, say, for an elliptic operator $P(x, D)$. As, however, the inequality is supposed to hold for *arbitrarily* large parameters of $\tau \geq \tau_0$, it turns out to be more challenging. In fact, the parameter τ plays the same role as a derivative (microlocally this can be made rigorous).

Let us describe the general strategy of proving an (L^2 -) Carleman estimate, in order to get a feeling for these inequalities. It consists of three key steps:

1. **Conjugation:** As it is difficult to prove an exponentially weighted estimate, it is more convenient to switch to the function $w = e^{\phi(x,\tau)} u$. Thus, the right hand side of the inequality (1.0.1) turns into

$$\left\| (e^{\phi(x,\tau)} P(x, D) e^{-\phi(x,\tau)}) w \right\|_{L^2(\Omega)}.$$

Hence, it becomes necessary to understand the conjugated operator

$$L_\phi := e^{\phi(x,\tau)} P(x, D) e^{-\phi(x,\tau)}.$$

2. **Pseudoconvexity Analysis:** Even for elliptic operators, after conjugation, the operator $L_\phi = e^{\phi(x,\tau)} P(x, D) e^{-\phi(x,\tau)}$ loses its ellipticity properties in general. Hence, it is not immediately clear how to obtain the desired lower bounds. In order to understand the origin of these lower bounds, we separate the symmetric and antisymmetric parts of the operator. Since the characteristic set of these is non-empty in general, a phase-space analysis demonstrates that on this set positivity – which is necessary for the existence of lower bounds – can only be achieved via the commutator (or in microlocal language: the Poisson bracket). Hence, it is necessary to show that this contribution is positive/ non-negative (for limiting Carleman weights) on the respective characteristic sets. This leads to a so-called *pseudoconvexity* condition that has to be satisfied on the intersection of the characteristic sets of the symmetric and

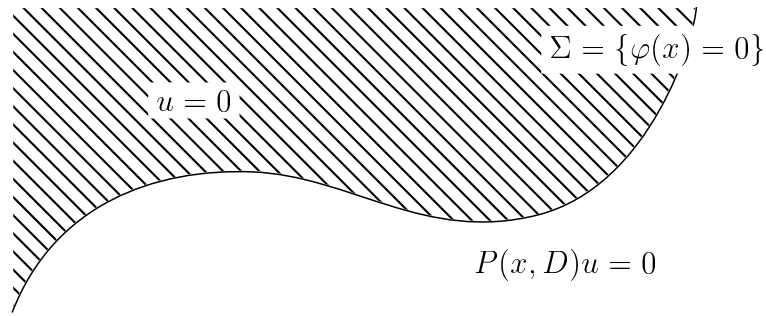


Figure 1.3: A (weak) unique continuation problem. For a general differential operator $P(x, D)$ one tries to transport information across a surface Σ . If the surface is strongly pseudoconvex with respect to the operator, it is possible to deduce $u \equiv 0$ globally. There is an intimate relation between pseudoconvex surfaces and the notion of pseudoconvexity of the corresponding weight functions.

antisymmetric parts of the operator.

3. **Choice of a Pseudoconvex Weight Function:** The analysis of the commutator/ Poisson bracket implies conditions on the weight function ϕ . Hence, the final step consists of finding an appropriate weight satisfying these conditions.

In the sequel, we carry out such an analysis for both elliptic and parabolic, local and non-local operators.

Results of the Thesis

In the following two chapters we present our main results on the previously presented questions. The main novelties here are an

- **Improved understanding of the “large angle regime” for the two-dimensional backward uniqueness problem for the heat equation.** In two dimensions we give a microlocal analysis of the backward uniqueness problem based on Carleman estimates. Here, we extend the minimal angle up to which the backward uniqueness property holds significantly (reaching opening angles of approximately 95°). We derive a simplified pseudoconvexity condition for one-dimensional Carleman weights which we evaluate numerically. This suggests that as far as one-dimensional Carleman weights are concerned, the angles which we reach are (nearly) optimal. Under additional vanishing assumptions we prove the backward uniqueness property for conical domains with opening angles larger than the critical 90° .
- **Improved understanding of unique continuation properties for fractional Schrödinger operators.** Via a Carleman based approach we prove the strong unique continuation property for fractional Schrödinger equations, thus complementing and improving various previous results from the literature. We rely on an argument in the spirit of Koch and Tataru [KT01a]. In

this way we can treat arbitrarily large scaling-critical potentials (with lower order perturbations) under low regularity assumptions. Furthermore, in the one-dimensional case we give a full characterization of the spectrum of a certain (degenerate) elliptic operator which allows to treat arbitrary potentials which are bounded by scaling-critical Hardy-potentials. Thus, we prove a result in the spirit of the work of Pan and Wolff [PW98].

Let us finally comment on the organization of the remainder of this first part of the thesis: In Chapter 2 we will deal with the backward uniqueness property of the heat equation while Chapter 3 is dedicated to the understanding of the unique continuation property of the non-local fractional Laplacian.

Chapter 2

Backward Uniqueness Properties of the Heat Equation in Unbounded Domains

2.1 Introduction

In the sequel we will be concerned with controllability properties of the heat equation. More precisely, we will focus on the so-called “backward uniqueness property” for the heat equation. This deals with the question of whether the prescription of final data determines a solution of the heat equation uniquely. Does

$$\begin{aligned}(\partial_t - \Delta)u &= Vu + W \cdot \nabla u \text{ in } \Omega \times (0, 1), \\ u(t = 1, x) &= 0 \text{ in } \Omega,\end{aligned}\tag{2.1.1}$$

already imply $u \equiv 0$ in $\Omega \times (0, 1)$ for appropriate choices of the potentials V and W ? The validity of the backward uniqueness property would, in particular, entail that there are no nontrivial initial and boundary data such that u satisfies (2.1.1). Due to the linearity of the heat equation such a phenomenon can be interpreted “causally”: Only a single choice of data can lead to a specific final state of a system if it is evolved by the heat equation. In other words, the “final state determines its past”. This would, for example, effect that if the temperature distributions of two objects agree at a given time, the history of the temperature distributions must have been identical at all previous times. From physical experience, e.g. heating a plate, one would not expect such a behaviour (for objects of finite size).

The “opposite” extreme situation is given by (boundary) “controllability”: Here, one poses the question whether it is possible to enforce a specific desired final temperature distribution (for instance $u(t = 1, x) = 0$) starting from a given initial

temperature distribution (in appropriate function spaces) via adapted boundary data. Examples of situations in which such a behaviour would be desirable are, for instance, the heating of a room so as to obtain a particularly comfortable temperature distribution or the heating of a chemically reacting substance from the boundary so as to control the respective reaction.

As we will see these properties strongly depend on the (un-)boundedness of the underlying domain.

In *bounded* domains these issues have been investigated thoroughly, c.f. [LRL11], [Zua07], [Zua06], [FR71], [Rus78], [TT11]. Choosing appropriate function spaces, it is possible to derive (boundary) null-controllability in this situation. This strongly agrees with our physical intuition. Mathematically, these results build on various approaches relying on Carleman estimates, spectral estimates, the method of moments and observability inequalities.

In the case of *unbounded* domains the situation is less transparent. In searching for controllability properties of the heat equation in unbounded domains, one might be tempted to recall the infinite speed of propagation of the heat equation as well as its strong diffusivity as indicators in favour of null-controllability. As a consequence, one might hope for null-controllability in spite of the unboundedness of the domain. On a second thought, however, this impression might be reversed by thinking of the *finite* “mean speed of propagation” – i.e. the finite speed with which a Gaussian diffuses in time. Whereas bounded domains do not “feel” this effect, it presents a serious issue in the case of unbounded domains.

In fact, it turns out that the unbounded setting differs qualitatively from the bounded one. We concentrate on unbounded, conical domains. There are two regimes:

- In the case of “small” angles ($\theta < 90^\circ$) there are initial data which can be driven to zero (“null-controllable initial data”).
- For large angles, it is impossible to diffuse the information from the boundary into the interior sufficiently fast.

Although reasonable heuristics suggest that the critical angle which distinguishes between these regimes should be given by exactly $\theta = 90^\circ$, there are no rigorous proofs for this. In the sequel we are mainly concerned with the “large angle regime”, pushing the upper bound closer to the conjectured 90° in the two-dimensional situation.

Mathematically, this regime is particularly interesting as most of the known technical tools break down: At first sight it seems impossible to obtain an expansion into a basis of eigenfunctions for the underlying elliptic operator, observability inequalities fail in general and Carleman estimates become much more restrictive as growth assumptions at infinity have to be satisfied. Yet, there are various partial results

on the “large angle regime”, c.f. [LŠ10], [MZ01a], [MZ01b], [Mil05]. The strongest previous result can be found in the paper by Li and Šverák [LŠ10] who employ Carleman techniques to derive the backward uniqueness property for heat equations with lower order terms in domains with opening angles of down to approximately 109° . However, the underlying Carleman weight does not have sufficient convexity properties in order to carry the estimate beyond this number.

In this chapter, we present two approaches dealing with the control problem in the “large angle regime”: While the first approach is very direct and highlights the difficulties in treating the backward uniqueness problem in conical domains, it mainly serves as a motivation for our main, more abstract approach via Carleman inequalities:

- **Exponential Estimates.** Our first approach is related to the papers [MZ01a], [MZ01b] by Zuazua and Micu and provides some intuition on the interplay between strong diffusion and possible cancellations. Its central tool consists of the method of moments. As in the articles by Zuazua and Micu, we derive a family of exponentially weighted estimates for the (L^2) boundary controlled heat equation. However, instead of obtaining the estimates via spectral properties of the operator in exponentially weighted spaces, we choose a direct approach via the Fourier transform. Although the approach is limited to certain very specific lower order perturbations, it provides good intuition for the problem and indicates that one can expect a continuum of exponential bounds and not only countably many as the spectral approach suggests. For “separable” boundary data this approach “explains” the special role of the angle of 90° .
- **Carleman Estimates.** In our second – and main – approach, we rely on the more abstract method of Šverák and Li [LŠ10] and prove Carleman estimates, c.f. also [ESŠ03]. Motivated by limiting Carleman weights for the Laplacian in two-dimensions, c.f. [KSU07], we carry out a pseudoconvexity analysis of the problem. Hence, we are able to improve the angular dependence in the two-dimensional situation: Investigating the necessary properties of Carleman weights, it is possible to give a condition guaranteeing pseudoconvexity – i.e. admissibility – for a larger class of weight functions in two-dimensional domains. With these it is possible to reach angles of (slightly) less than 95° in two dimensions.

Let us comment a little bit further on the Carleman approach. The guiding intuition behind these estimates is provided by the time-independent setting: For lower order perturbations of the Laplacian, Carleman estimates hold down to an angle of 90° in the two-dimensional case. Thus, these estimates provide backward uniqueness for the heat equation if additionally $u(0, \cdot) = 0$ is assumed (c.f. Proposition 8). In particular, this proves that if certain initial data for the parabolic equation were null-controllable, then the corresponding (boundary) control would necessarily

be unique. However, the general case – i.e. the full proof of the backward uniqueness result – is much more difficult to handle, as the very convenient orthogonality relation on the characteristic set in the spatial variables is lost: While in phase space the characteristic set of the elliptic symbol is given by the intersection of a circle with the plane normal to $\nabla\phi$, in the full parabolic setting it is given by the intersection with the same circle and arbitrary (time frequency) translations of the described plane. This causes new challenges in understanding the combination of the underlying geometry and convexity conditions.

Our choice of the weight function is essentially one-dimensional. We believe that for this class the weights we use are (nearly) optimal. In order to improve the angle further (towards the conjectured 90°), one would have to find a new two-dimensional class of functions. However, it is not immediately clear how this might be achieved.

We briefly indicate the organization of the remainder of the chapter: In the next section we recall some basic notions from control theory. With this background, it is possible to review the previously existing results, indicate certain central arguments and explain their relation to our problem (Section 2.2). In Section 2.3 we present the derivation of exponential bounds. These can be interpreted as heuristics indicating that the critical angle should indeed be given by 90° . We state our main results in Section 2.4. The proofs are then presented in Sections 2.5 and 2.6: Here, we prove the elliptic (Section 2.5) and parabolic (Section 2.6) Carleman estimates which imply the backward uniqueness property.

2.2 Review: (Non-)Controllability – Definitions, Basic Properties and Examples from the Literature

In this section we briefly recall some of the central notions used in control theory. As the equivalence of the observability and null-controllability properties presents a key element of control theory (for the heat equation), we include a short proof. We only formulate the results in the setting of the linear heat equation. However, generalizations to lower order perturbations can be treated along the same lines. We follow the review article of Zuazua [Zua07].

Different Notions of Controllability

In the sequel we recall some of the most commonly used notions of controllability.

Definition 1 (Notions of Controllability). *Let $\Omega \subset \mathbb{R}^n$ and let $u : \Omega \times [0, T] \rightarrow \mathbb{R}$ be a solution of the heat equation*

$$(\partial_t - \Delta)u = 0 \text{ in } \Omega \times (0, T). \quad (2.2.1)$$

- The equation (2.2.1) is (boundary) null-controllable if for all initial data $u_0 : \Omega \rightarrow \mathbb{R}$, $u_0 \in L^2(\Omega)$, there exist boundary controls $f : \partial\Omega \times [0, T] \rightarrow \mathbb{R}$, $f \in L^2(\partial\Omega \times [0, T])$, such that $u(T, x) = 0$ for all $x \in \Omega$.
- Initial data $u_0(x) \in L^2(\Omega)$ are (boundary) null-controllable if there exist boundary controls $f : \partial\Omega \times [0, T] \rightarrow \mathbb{R}$, $f \in L^2(\partial\Omega \times [0, T])$, such that $u(T, x) = 0$ for all $x \in \Omega$.

Remark 1. • Due to the smoothing effect of the heat equation it is not possible to reach arbitrary final data $u_T \in L^2(\Omega)$ via $L^2(\partial\Omega)$ boundary controls, in this sense the equation is “not controllable”.

- As a consequence of the linearity of the equation, the null-controllability property implies controllability for any other datum in $e^{T\Delta}L^2$ (that is the image under the heat semi-group with zero boundary data).

Definition 2 (Adjoint System). *Let $\varphi : \Omega \times [0, T] \rightarrow \mathbb{R}$. It satisfies the adjoint problem to the heat equation with final data φ_T if it solves*

$$\begin{aligned} (\partial_t + \Delta)\varphi &= 0 \text{ in } \Omega \times [0, T], \\ \varphi &= 0 \text{ on } \partial\Omega \times [0, T], \\ \varphi &= \varphi_T \text{ on } \Omega \times \{T\}. \end{aligned} \tag{Adjoint}$$

Remark 2. As can be seen from the definition, the adjoint heat equation is well-posed in L^2 : By a reflection in time it turns into the standard heat equation with zero boundary data.

Definition 3 (Approximate Controllability). *The equation (2.2.1) is approximately controllable if for any initial datum $u_0 \in L^2(\Omega)$ the set of reachable states is dense in $L^2(\Omega)$, i.e. $\{u \in L^2(\Omega) \mid \exists f : \partial\Omega \times [0, T] \rightarrow \mathbb{R}, f \in L^2(\partial\Omega \times [0, T]) \text{ such that } u = e_f^{T\Delta}u_0\}$ is dense in $L^2(\Omega)$, where the subscript f denotes the heat semi-group with boundary data f .*

Remark 3. The approximate controllability property can be related to unique continuation properties of the adjoint problem. Thus, there is an intimate relation to Holmgren’s theorem, c.f. [Zua06].

Definition 4 (Backward Uniqueness). *The heat equation satisfies the backward uniqueness property (BUP) in the domain Ω if all solutions $u : \Omega \times [0, T] \rightarrow \mathbb{R}$ of (2.2.1) with $u(T, x) = 0$ and $\|u\|_{L^\infty(\Omega \times [0, T])} < \infty$ already vanish identically, i.e. $u \equiv 0$ in $\Omega \times [0, T]$.*

It is interesting to observe the different degrees of “controllability”. Whereas the heat equation is only null-controllable in *bounded* domains, it is only approximately controllable in any (sufficiently regular) domain, c.f. [DT98].

Last but not least, we recall the following quantitative characterization of null-controllability, [Zua07]:

Proposition 2 (Equivalence of Null-Controllability and Observability, [Zua07]). *The heat equation is (boundary) null-controllable (in L^2) iff an observability inequality holds, i.e. for any solution $\varphi : \Omega \times [0, T] \rightarrow \mathbb{R}$ of the adjoint equation associated with an arbitrary final datum $\varphi_T \in L^2(\Omega)$ the inequality*

$$\|\varphi(0, \cdot)\|_{L^2(\Omega)}^2 \leq C_T \int_0^T \int_{\partial\Omega} |\partial_n \varphi(t, x)|^2 d\mathcal{H}^{n-1}(x) dt \quad (2.2.2)$$

holds.

It is important to note that in the observability inequality the initial data of the adjoint equation are controlled by *boundary* contributions. Hence, the estimate is highly nontrivial in general. In particular, it is not merely a consequence of the regularization provided by the heat equation.

In demonstrating that null-controllability cannot hold (for general L^2 data), it therefore suffices to prove that the observability inequality (2.2.2) does not hold true. However, this does not rule out controllability in weighted spaces. Furthermore, it also does not exclude the possibility of specific data being null-controllable.

Review of the Literature on the (Non-)Controllability Properties of the Heat Equation in Unbounded Domains

In this section we briefly review the literature on (non-)controllability properties of the heat equation in certain unbounded domains. We focus on conical domains. As these are obtained as blow-ups of (bounded) Lipschitz domains, it is of special interest to understand the behaviour of the heat equation from a control theoretic point of view on these.

- **The whole space.** The whole space situation is a classical result. For the heat equation without lower order terms, the backward uniqueness property can be proved by a reduction to an ODE in Fourier space. Via Carleman estimates or alternative forms of convexity estimates, e.g. logarithmic convexity [AN67], it is possible to extend this to the case of general uniformly elliptic operators with lower order terms, c.f. [Fri64].
- **The half space.** The controllability properties of the heat equation in the half space were considered by Micu & Zuazua [MZ01a], [MZ01b] in the context of control theory. Using the method of moments, the authors prove the backward uniqueness property in arbitrary (negative) H^s spaces. They complement this with the observation that in spaces with exponentially growing (generalized Fourier-) modes it is possible to find null-controllable (initial) data.

As certain uniqueness questions for the Navier-Stokes equations can be reduced to a backward uniqueness statement for the heat equation, c.f. [SŠ02],

Seregin and Šverák began to investigate the backward uniqueness properties of this equation. Together with Escauriaza [ESŠ03], they employ techniques originating from the field of unique continuation in order to derive the backward uniqueness property in the half space.

- **Conical Domains with Opening Angles $\theta \geq 109^\circ$.** The ideas from [ESŠ03] were further pursued in a paper by Šverák & Li [LŠ10], who deal with conical domains with opening angles strictly less than 180° . Again, the main results are based on Carleman estimates.

As discussed in Section 2.4, our results rely on similar techniques as the ones of Šverák et al. However, we make stronger use of the *microlocal* interpretation of Carleman estimates which allows us to deduce necessary conditions for the Carleman weight. Via pseudoconvexity conditions we obtain a phase space differential inequality. Hence, it becomes easier to derive appropriate weight functions via “educated guesses”.

Characteristic Examples from the Literature

Last but not least, we review four examples in order to obtain an intuition for the control problem in unbounded domains. Furthermore, we recall an elliptic non-existence result which serves as a model situation for the backward uniqueness property of the heat equation.

- The first example recalls a fundamental result of Lebeau and Robbiano, c.f. [LR95], stating that in *bounded* domains the heat equation is null-controllable. In briefly outlining a possible proof of the argument – we follow the presentation of Lebeau and Le Rousseau [LRL11] – it is possible to identify the strong diffusivity of the heat equations as a key reason of the null-controllability property in bounded domains. The techniques of the proof indicate the relevance of the boundedness of the domain.
- With the second example, which is an argument due to Zuazua and Micu [MZ01a], [MZ01b], we demonstrate that the difference between bounded and unbounded domains is not merely an artifact of the techniques, but an *intrinsic* property. In unbounded domains the observability inequality (2.2.2) fails. Therefore one *cannot hope for null-controllability* properties (in unweighted spaces).
- Moreover, we present Escauriaza’s example of a caloric function which is null-controllable in a conical domain with a sufficiently small opening angle. This shows that for small angles it is not possible to extrapolate from the whole space situation: In domains with small opening angles the backward uniqueness property is not satisfied.
- Finally, we prove that there is no harmonic function with Gaussian decay in an angular domain with an opening angle $\theta \geq \frac{\pi}{2}$. Combined with the

decay properties of caloric functions which are assumed to be null-controllable (c.f. Lemma 5), this indicates that the elliptic equation provides the “right” intuition for its parabolic analogue.

These examples highlight that for the “small angle regime” neither controllability (in unweighted spaces) nor the backward uniqueness property holds in unbounded conical domains. However, the elliptic non-existence result suggests that in the “large angle regime” – the Phragmen-Lindelöf principle provides the threshold – the backward uniqueness property is satisfied.

Null-Controllability of the Heat Equation in Bounded Domains

In bounded domains we have the following central result due to Lebeau and Robbiano [LR95]:

Theorem 1 (Lebeau, Robbiano, [LR95]). *Let $\Omega \subset \mathbb{R}^n$ be a bounded domain. Then the heat equation is null-controllable from the boundary, i.e. for any $u_0 \in L^2(\Omega)$ there exists a boundary control $f \in L^2(\partial\Omega \times [0, T])$ such that*

$$\begin{aligned} (\partial_t - \Delta)u &= 0 \text{ in } \Omega \times (0, T), \\ u &= f \text{ on } \partial\Omega \times [0, T], \\ u &= u_0 \text{ on } \Omega \times \{0\}, \\ u &= 0 \text{ on } \Omega \times \{T\}. \end{aligned}$$

We briefly sketch the argument following Lebeau and Le Rousseau [LRL11]. The proof relies on two key ingredients: A spectral estimate for the Dirichlet Laplacian as well as a resulting observability inequality for a “finite-dimensional” control problem. For a finite number of eigenfunctions, one has the following sharp bound:

Theorem 2 (Lebeau, Robbiano, [LR95]). *Let $\Omega \subset \mathbb{R}^n$ be bounded. Let ϕ_j be an eigenfunction of the Dirichlet Laplacian on Ω , corresponding to the eigenvalue μ_j . Then we have*

$$\left\| \sum_{\mu_j \leq \mu} \alpha_j \phi_j \right\|_{L^2(\Omega)}^2 \leq K e^{K\sqrt{\mu}} \left\| \sum_{\mu_j \leq \mu} \alpha_j \partial_n \phi_j \right\|_{L^2(\partial\Omega)}^2. \quad (2.2.3)$$

The crucial observation here is that the boundary data – i.e. functions whose support lies in a set of lower Hausdorff-dimension – control the bulk contributions. Hence, there cannot be “too bad” cancellations on the boundary. Although the original full orthogonality of the ϕ_j is lost, part of it is “inherited” by the boundary contributions. The sharpness of this estimate can be observed by considering the flow of eigenfunctions with the heat semi-group and using Weyl’s law.

Arguing via duality, it is then possible to prove a partial control result, i.e. a control result in a finite-dimensional space spanned by a finite number of eigenfunctions

associated with the Laplacian, and an exponential estimate on the L^2 norm of the boundary control. As a consequence of (2.2.3), the exponential factor involved in the estimate only grows with the square root of the highest frequency.

Finally, this implies the desired controllability property, as it is now possible to iteratively “project away” eigenmodes for any given initial datum. Combined with a “relaxation phase” in which the strong diffusivity of the heat equation serves to control the loss in the constant of the observability inequality, this entails the desired result.

The detailed discussion of this (central) proof is instructive in highlighting mechanisms that distinguish the bounded and the unbounded situation. The crucial ingredient, estimate (2.2.3), does not have an appropriate analogue in the unbounded situation. Although it is possible to understand the notion of eigenvalues and eigenfunctions in an appropriate sense, such a strong bound cannot be obtained. In a sense, the diffusivity is not strong enough to counteract the unboundedness of the domain.

Lack of Null-Controllability

In the literature there is good reason indicating that the behaviour of solutions of the heat equation in *unbounded* domains has to differ strongly from that in *bounded* domains. In an unbounded domain it is not possible to expect that the heat equation satisfies an observability inequality. As Micu and Zuazua [MZ01a] point out, a simple translation argument proves that this cannot be possible without an additional weight: Our starting point is the equivalence of the null-controllability property (in L^2) with an observability inequality for the adjoint system. In the half-space, \mathbb{R}_+^n , this amounts to

$$\|\varphi(0)\|_{L^2(\mathbb{R}_+^n)}^2 \leq C \int_0^T \int_{\mathbb{R}^{n-1}} \left| \frac{\partial \varphi}{\partial x_n} \right|^2 dx' dt,$$

where φ satisfies the adjoint heat equation with final data φ_T . Considering $\varphi_T \in C_0^\infty(\Omega)$, $\varphi_T \geq 0$, we define translations $\varphi_{T,k}(x) := \varphi_T(x - ke_n)$. Then the boundary integral decreases exponentially, while the L^2 norm of the initial data does not decrease for a sequence of sufficiently large k . As a result the observability inequality cannot hold in general.

This heuristic argument (which can be adapted to an arbitrary cone) suggests that the heat equation behaves differently in unbounded domains; yet it does not prove the non-existence of (boundary) null-controllable initial data.

Escauriaza’s Example

We briefly recall Escauriaza’s example, c.f. [LŠ10]: It proves that in cones with sufficiently small opening angles it is possible to find null-controllable initial data.

Considering the remaining variables as dummy variables, it suffices to provide an example in two dimensions only. For that purpose we introduce the Appell transform. This is a symmetry transform of the heat equation in conical domains: It allows to switch from a solution, $u(x, t)$, of the forward heat equation to a solution, $v(y, s)$, of the backward heat equation. In particular, it can be employed in order to transform a harmonic function into the desired example. Assume that v is a solution of the backward heat equation

$$(\partial_t + \Delta)v = 0 \text{ in } \Omega_\theta \times (0, T),$$

where Ω_θ is a cone with opening angle θ . Then the (two-dimensional version of the) Appell transform is given by

$$u(x, t) = \frac{1}{4\pi t} e^{-\frac{|x|^2}{4t}} v\left(\frac{x}{t}, \frac{1}{t}\right).$$

It turns the backward caloric function v into the caloric function u and vice versa. In particular, starting with a harmonic function, h , it becomes possible to associate a backward caloric function, v , to it via Appell's transform. We consider the harmonic function

$$h(x) = \Re(e^{-(x_1 + ix_2)^\alpha}), \quad \alpha > 2.$$

An application of Appell's transform yields a solution of

$$\begin{aligned} \partial_t v + \Delta v &= 0 \text{ in } \Omega_\theta \times (0, 1), \\ v &= 0 \text{ in } (\Omega_\theta \times \{0\}) \setminus \{(0, 0)\}. \end{aligned}$$

Explicitly, it is given by

$$v(x, t) = \frac{4\pi}{t} e^{\frac{|x|^2}{4t}} h\left(\frac{x}{t}\right).$$

Away from the (spatial) origin, this function is uniformly bounded in any cone of angle $\theta \in [0, \frac{\pi}{\alpha}]$. Thus, translating in space and reflecting in time yields a counterexample to the backward uniqueness property of the heat equation, i.e.

$$u(x, t) = v(x_1 + 1, x_2 + 1, 1 - t).$$

satisfies

$$\begin{aligned} (\partial_t - \Delta)u &= 0 \text{ in } \Omega_\theta \times (0, 1), \\ u &= 0 \text{ in } \Omega_\theta \times \{1\}, \\ |u| &\leq C \text{ in } \Omega_\theta \times [0, 1]. \end{aligned}$$

Remark 4. We point out that Escauriaza's example of the failure of the backward

uniqueness property is limited to cones with opening angles strictly less than $\frac{\pi}{2}$. This follows from the growth condition imposed on complex analytic functions by the Phragmen-Lindelöf principle. As we will see in the next section, there are no nontrivial harmonic functions with a Gaussian decay rate in cones with opening angles greater than or equal to $\frac{\pi}{2}$.

Excursion: Non-Existence Results for Harmonic Functions with Gaussian Decay Rates in 2D Cones

The non-existence of harmonic functions with Gaussian decay in 2D cones can be derived via various methods such as elliptic Carleman inequalities or comparison principles in unbounded domains (Phragmen-Lindelöf principles). In the sequel we present a first proof of this non-existence result in cones of an opening angle greater or equal to $\frac{\pi}{2}$ in two dimensions. We employ the complex Phragmen-Lindelöf principle; later we provide a more stable proof via Carleman estimates (c.f. Section 2.5).

Proposition 3. *Let $\Omega_\theta \subset \mathbb{R}^2$ be a conical domain. Then there exist (nontrivial) harmonic functions decaying with an at least Gaussian rate if and only if $\theta < \frac{\pi}{2}$.*

For our proof we argue similarly as in Li [Li11]. As Li, we rely on the holomorphic Phragmen-Lindelöf Theorem which is considerably stronger than the analogue for harmonic functions (as both real and imaginary part have to satisfy the theorem):

Theorem 3 (holomorphic Phragmen-Lindelöf, [Mar77]). *Let G be the interior of a cone with opening angle of $\alpha\pi$ radians ($0 < \alpha \leq 2$) with boundary Γ , and let $f(z)$ be a complex analytic function in G , continuous up to the boundary. Suppose $f(z)$ satisfies*

$$(i) \quad f(z) \leq C < \infty \text{ on } \Gamma,$$

$$(ii) \quad \liminf_{r \rightarrow \infty} \frac{\ln M(r)}{r^\alpha} \leq 0 \text{ where } M(r) = \sup_{|z|=r, z \in G} |f(z)|.$$

Then $|f(z)| \leq C$.

With this, we can carry out the proof of the non-existence proposition.

Proof of Proposition 3. Existence follows from choosing the real part of the holomorphic function which was already used in Escauriaza's example:

$$u(x_1, x_2) = \Re(e^{(x_1 + ix_2)^\alpha}),$$

where $\alpha > \frac{\pi}{\theta}$.

Thus, it remains to prove the non-existence of harmonic functions with a Gaussian decay rate in cones with opening angles larger than or equal to $\frac{\pi}{2}$. Here, it suffices to argue that no such function exists in a cone of angle precisely $\frac{\pi}{2}$, as this implies the result on cones with larger angles by restriction.

We argue by contradiction. Assume that we had a harmonic function with Gaussian decay in $\mathbb{R}_+ \times \mathbb{R}_+$. By an even reflection this can be extended to a function on the whole space solving

$$\Delta u = \delta_{\{x=0\}}f(y) + \delta_{\{y=0\}}g(x), \tag{2.2.4}$$

where $f = 2 \lim_{x \rightarrow 0} \frac{\partial}{\partial y} u(x, y)$ and $g = 2 \lim_{y \rightarrow 0} \frac{\partial}{\partial x} u(x, y)$. From the Gaussian decay we deduce that the Fourier transform of u and ∇u is bounded exponentially:

$$\mathcal{F}u(k) \leq C e^{\Im(k)^2}. \tag{2.2.5}$$

Therefore, it can be extended as a holomorphic function in each of its variables. The same is true for $\mathcal{F}f$ and $\mathcal{F}g$. Furthermore, in Fourier space the equation reads

$$(k_1^2 + k_2^2)\mathcal{F}u(k_1, k_2) = \mathcal{F}f(k_2) + \mathcal{F}g(k_1).$$

On the real axis both functions $\mathcal{F}f, \mathcal{F}g$ are bounded and decay to zero. In order to derive decay along the imaginary axis, we set $k_1 = ik = ik_2$. Inserted into (2.2.4), this leads to

$$0 = \mathcal{F}f(ik) + \mathcal{F}g(k).$$

Thus $\mathcal{F}f$ and $\mathcal{F}g$ are also bounded on the imaginary axis. Now, we would like to apply the Phragmen-Lindelöf theorem, the bound $e^{|k|^2}$, however, is insufficient in the cone of angle $\frac{\pi}{2}$. Nevertheless, with an idea of Li [Li11], it is possible to uniformly apply the Phragmen-Lindelöf theorem in smaller angles tending to the full angle. More precisely, consider the function $\mathcal{F}f$ on

$$G_\theta := \left\{ z \in \mathbb{C} \text{ s.t. } 0 < \theta < \arg(z) < \frac{\pi}{2} \right\}.$$

For any θ , it is possible to find $\sigma(\theta) > 0$ with $\sigma(\theta) \rightarrow 0$ as $\theta \rightarrow 0$, such that $\tilde{f} := e^{i\sigma(\theta)z^2}\mathcal{F}f$ is uniformly (independently of the angle θ) bounded on the boundary of G_θ . This follows from the bound (2.2.5) in terms of the imaginary part only. As this auxiliary function further satisfies $|\tilde{f}(k)| \leq C e^{|k|^2}$, the Phragmen-Lindelöf theorem on the smaller conical domain G_θ implies $|\tilde{f}| < C$ uniformly in $\theta \rightarrow 0$. In the limit $\theta \rightarrow 0$ and $\sigma \rightarrow 0$, this reduces to $|\mathcal{F}f| \leq C$ in the first quadrant. Analogously, the statement holds in any quadrant. Therefore, Liouville's theorem yields $\mathcal{F}f, \mathcal{F}g \equiv 0$. Finally, this also implies $\mathcal{F}u = 0$. □

2.3 Heuristics for the Backward Uniqueness Property and Derivation of Exponential Bounds for Null-Controllable Solutions

In this section we recover the results of Zuazua and Micu [MZ01a], [MZ01b] in the setting of the heat equation without lower order perturbation terms via very direct methods. This serves a two-fold purpose:

- On the one hand, the behaviour of the heat equation becomes more transparent than in the relatively abstract Carleman approach which is pursued in the later sections. In choosing this direct approach via the explicit form of the fundamental solution, the difficulties in dealing with the backward uniqueness property are clarified. In this sense, the direct approach can be considered as heuristics for the later, more abstract treatment.
- On the other hand, the results as such are already interesting. Although we use similar techniques as Micu and Zuazua [MZ01a], [MZ01b] the crucial estimates – our exponential bounds – are derived in a more direct manner than theirs (which is also due to the fact that Micu and Zuazua aim at understanding very rough solutions). The restriction to a special class of boundary data highlights the critical role of the angle $\theta = \frac{\pi}{2}$.

In terms of the backward uniqueness property, the main result of this section is the following null-controllability result for “separable data” (which is an intrinsic feature of the *unbounded* situation):

Proposition 4. *Let $g_1(x_1, t) = g_{11}(x_1)g_{12}(t) \in L^2(\mathbb{R}_+ \times [0, T]) \cap L^1(\mathbb{R}_+ \times [0, T])$ and $g_2(x_2, t) = g_{21}(x_2)g_{22}(t) \in L^2(\mathbb{R}_+ \times [0, T]) \cap L^1(\mathbb{R}_+ \times [0, T])$. Assume that $u_0 \in L^2(\mathbb{R}_+ \times \mathbb{R}_+) \cap L^1(\mathbb{R}_+ \times \mathbb{R}_+)$ and that*

$$\begin{aligned}
 (\partial_t - \Delta)u &= 0 \text{ in } (\mathbb{R}_+ \times \mathbb{R}_+) \times (0, T), \\
 u &= g_1 \text{ on } \mathbb{R}_+ \times \{x_2 = 0\} \times [0, T], \\
 u &= g_2 \text{ on } \{x_1 = 0\} \times \mathbb{R}_+ \times [0, T], \\
 u &= u_0 \text{ on } \mathbb{R}_+ \times \mathbb{R}_+ \times \{0\}, \\
 u &= 0 \text{ on } \mathbb{R}_+ \times \mathbb{R}_+ \times \{T\}.
 \end{aligned} \tag{2.3.1}$$

Then $u \equiv 0$ (and in particular $g_1, g_2 \equiv 0$).

In their articles on the backward uniqueness properties of the heat equation, Micu and Zuazua [MZ01a], [MZ01b] argue via an expansion into an eigenbasis of a “modified Laplacian”. Their method of proof can be summarized in two fundamental steps:

- **The derivation of bounds for sufficiently many exponentially weighted integrals.** The use of weighted norms compactifies the underlying elliptic operator after a suitable change of coordinates. Hence, it is possible to consider

an evolution driven by a self-adjoint, compact operator. In this setting the spectrum of the (spatial) operator can be determined explicitly. This allows to phrase the backward uniqueness question as a moment problem.

- **A Titchmarsh-like theorem (c.f. Lemma 3).** This second step implies that the boundary data and hence the function itself must already be identically zero. The argument leading to the desired claim can be interpreted as a quantification of the statement that if all moments of a function vanish, then this function is identically zero.

However, this approach seems to be restricted to the half-space setting or to classes of boundary data with additional structure (e.g. product structure), as otherwise oscillations play a relevant, not easily controlled role.

In the sequel the exponential bounds are derived as a consequence of the representation formula for the fundamental solution of the heat equation in the half-/quarter-space. This allows to recover Micu and Zuazua's bounds on exponentially weighted integrals of the boundary data. Although this ansatz is restricted to the unperturbed heat equation as well as a very limited scope of perturbations, compared to the original approach of Zuazua and Micu it has the advantage of providing a continuum of exponential bounds as one is not restricted to work with the discrete eigenvalues. Furthermore, the structure of the fundamental solution indicates that the case of an opening angle of 90° plays a special role.

Before proceeding with the proof of Proposition 4, we derive analogous statements for the one and higher-dimensional control problems in the half space. Thus, we recover the results of Zuazua and Micu.

The 1D case

Without invoking the decomposition into eigenstates, the argument of Micu & Zuazua [MZ01a] can be recovered by using the explicit form of the fundamental solution in the half-space case. We carry out the corresponding calculations in 1D first.

Lemma 1. *Let $u_0 : (0, \infty) \rightarrow \mathbb{R}$, $u_0 \in L^2((0, \infty)) \cap L^1((0, \infty))$, $g : [0, T] \rightarrow \mathbb{R}$, $g \in L^2([0, T])$ and let $u : (0, \infty) \times [0, T] \rightarrow \mathbb{R}$ satisfy*

$$\begin{aligned}
 (\partial_t - \Delta)u &= 0 \text{ in } (0, \infty) \times (0, T), \\
 u &= g \text{ on } \{0\} \times [0, T], \\
 u &= u_0 \text{ in } (0, \infty) \times \{0\}, \\
 u &= 0 \text{ in } (0, \infty) \times \{T\}.
 \end{aligned}
 \tag{2.3.2}$$

Then the following exponential bounds hold:

$$\left| \int_0^T e^{k^2 s} g(s) ds \right| \leq \frac{C}{|k|} \text{ for all } k \in \mathbb{R}. \quad (2.3.3)$$

Remark 5. As we will see from Lemma 5, the condition on the integrability – $u_0 \in L^2((0, \infty)) \cap L^1((0, \infty))$ – can be significantly relaxed.

Proof. Using the method of reflection (mirror charges), the Green's function, $G_{(0, \infty)}(x, y, t)$, of the one-dimensional heat equation in the half-space can be computed explicitly:

$$G_{(0, \infty)}(x, y, t) = \frac{1}{\sqrt{2\pi t}} \left(e^{-\frac{|y-x|^2}{4t}} - e^{-\frac{|y+x|^2}{4t}} \right).$$

As a consequence, the solutions of (2.3.2) can be represented as

$$u(x, t) = ((\partial_y G_{(0, \infty)})|_{y=0} *_t g)(x, t) + \int_{(0, \infty)} G_{(0, \infty)}(x, y, t) u_0(y) dy.$$

Extending the initial data by zero, this can be rephrased in terms of the standard heat kernel, $G(x, y, t) = G(x - y, t)$:

$$u(x, t) = 2((\partial_y G)|_{y=0} *_t g)(x, t) + (G *_x (Pu_0))(x, t),$$

where P is a reflection operator defined by

$$(Pw)(x) = w(x) - w(-x).$$

This yields a function which is caloric in $(0, \infty) \times (0, T]$ and belongs to $L^2(\mathbb{R}) \cap L^1(\mathbb{R})$ for almost every $t \in [0, T]$. Thus, it is possible to carry out a spatial Fourier transform:

$$\mathcal{F}u(x, t) = e^{-tk^2} \left(\mathcal{F}Pu_0(k) - k \int_0^t e^{k^2 s} g(s) ds \right),$$

Evaluating the expression at time $t = T$ and using the assumption that $u(x, T) = 0$, we obtain

$$\mathcal{F}Pu_0(k) = k \int_0^T e^{k^2 s} g(s) ds. \quad (2.3.4)$$

As $Pu_0 \in L^2(\mathbb{R}) \cap L^1(\mathbb{R})$, we have

$$|\mathcal{F}Pu_0(k)| \leq C < \infty.$$

Dividing both sides of (2.3.4) by k , yields the desired result. \square

This central bound being established, we proceed along the lines of Micu & Zuazua [MZ01a], using the following statements. For the convenience of the reader we include the proofs.

Lemma 2 (Micu & Zuazua, [MZ01a]). *Let $g \in L^2(0, T)$, $0 \leq t \leq T$. Then we have*

$$\lim_{x \rightarrow \infty} \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k!} \int_0^T e^{kx(t-u)} g(u) du = \int_0^t g(u) du.$$

Proof. The result follows from an application of the dominated convergence theorem combined with the identity

$$\sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k!} e^{kx(t-u)} = (-1)[e^{-e^{(t-u)x}} - 1].$$

□

Lemma 3 (Micu & Zuazua, [MZ01a]). *Let $g \in L^2(0, T)$ be such that there exist constants $\delta > 0, C_\delta > 0$ with*

$$\left| \int_0^T g(u) e^{mu} du \right| \leq C_\delta e^{m\delta} \text{ for all } m \geq 1. \quad (2.3.5)$$

Then $\text{supp}(g) \subset [0, \delta]$.

This lemma explains the term “method of moments”: By having sufficiently strong estimates on “generalized moments”, i.e. on scalar products with a sufficiently large family of weights, it is possible to deduce the desired uniqueness property.

Proof. For any $0 \leq t < T - \delta$ the previous lemma implies the identity

$$\int_0^t g(T-u) du = \lim_{m \rightarrow \infty} \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k!} \int_0^T e^{km(t-u)} g(T-u) du.$$

This expression can be bounded due to (2.3.5)

$$\begin{aligned} \left| \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k!} \int_0^T e^{km(t-u)} g(T-u) du \right| &\leq \sum_{k=1}^{\infty} \frac{1}{k!} e^{km(t-T)} \left| \int_0^T e^{km\tau} g(\tau) d\tau \right| \\ &\leq \sum_{k=1}^{\infty} \frac{1}{k!} e^{km(t-T)} C_\delta e^{km\delta} \\ &= C_\delta (\exp(e^{m(t-T+\delta)}) - 1). \end{aligned}$$

However, the last expression vanishes as $m \rightarrow \infty$. □

Combining the observations of Lemma 2 and 3, it is possible to deduce backward uniqueness of the one-dimensional heat equation in the half-space:

Proposition 5. Let $u_0 : (0, \infty) \rightarrow \mathbb{R}$, $u_0 \in L^2((0, \infty)) \cap L^1((0, \infty))$, $g : [0, T] \rightarrow \mathbb{R}$, $g \in L^2([0, T])$ and let $u : (0, \infty) \times [0, T] \rightarrow \mathbb{R}$ satisfy

$$\begin{aligned} (\partial_t - \Delta)u &= 0 \text{ in } (0, \infty) \times (0, T), \\ u &= g \text{ on } \{0\} \times [0, T], \\ u &= u_0 \text{ in } (0, \infty) \times \{0\}, \\ u &= 0 \text{ on } (0, \infty) \times \{T\}. \end{aligned} \tag{2.3.6}$$

Then $u \equiv 0$.

Proof. Due to the bounds (2.3.3) (applied to $k = \sqrt{n}$, for $n \in \mathbb{N} \setminus \{0\}$), it is possible to apply Lemma 3 for any $\delta > 0$. Due to the integrability of the solution of (2.3.6), this implies the result. \square

The Case \mathbb{R}_+^n : Reduction to the 1D Case

As in the argument of Zuazua and Micu [MZ01b], the case of the half-space can be reduced to the one-dimensional situation. With our strategy this turns out to be significantly easier than the original argument of Zuazua and Micu. Indeed, we may employ the simple one-dimensional strategy as presented above.

As before, the Green's function can be computed explicitly:

$$G(x, y, t) = \frac{1}{(4\pi t)^{\frac{n}{2}}} \left(e^{-\frac{|y-x|^2}{4t}} - e^{-\frac{|y-\tilde{x}|^2}{4t}} \right),$$

where $\tilde{x} = (x_1, \dots, x_{n-1}, -x_n)$.

Going through the same arguments as in the previous section, one obtains the following identity:

$$\mathcal{F}P u_0(k) = k_n \int_0^T e^{k^2 s} \mathcal{F}g(k_1, \dots, k_{n-1}, s) ds.$$

Fixing (k_1, \dots, k_{n-1}) and considering a sequence $\{k_n^m\}_{m \in \mathbb{N}}$, $k_n^m \rightarrow \infty$, again yields exponential bounds comparable to those in (2.3.3). By an application of the Titchmarsh-like result of Lemma 3, we infer the backward uniqueness property.

The Case $\mathbb{R}_+ \times \mathbb{R}_+$: Uniqueness in the Class of Product Boundary Data – Proof of Proposition 4

In the sequel we investigate the (two-dimensional) control problem involving boundary data which separate in the temporal and spatial variables, i.e.

$$g_i(x_i, t) = g_{i1}(x_i)g_{i2}(t),$$

with $i \in \{1, 2\}$. Similar to the results in [MZ06], this additional restriction allows to prove the backward uniqueness property for the heat equation restricted to this

class of boundary data in $\mathbb{R}_+ \times \mathbb{R}_+$. In order to prove Proposition 4, we derive a representation formula for solutions of (2.3.1):

Lemma 4. *Let $u : (\mathbb{R}_+ \times \mathbb{R}_+) \times [0, T] \rightarrow \mathbb{R}$ be a solution of (2.3.1). Then it has the representation*

$$\begin{aligned} u(x, t) = & (G *_x (Pu_0))(x, t) + 2(\partial_{y_2} G \Big|_{y_2=0} *_x *_{x_1, t} P g_1)(x, t) \\ & + 2(\partial_{y_1} G \Big|_{y_1=0} *_x *_{x_2, t} P g_2)(x, t), \end{aligned} \quad (2.3.7)$$

where G denotes the standard whole space fundamental solution and P denotes the reflection operator $(Pu)(x_1, x_2) = u(x_1, x_2) - u(-x_1, x_2) - u(x_1, -x_2) + u(-x_1, -x_2)$. Furthermore, we obtain the Fourier representation

$$\begin{aligned} \frac{\mathcal{F}u(k, t)}{k_1 k_2} = & - \int_0^T e^{-k^2(t-s)} \left(\frac{\mathcal{F}(\tilde{P}g_1)(k_1, s)}{k_1} + \frac{\mathcal{F}(\tilde{P}g_2)(k_2, s)}{k_2} \right) ds \\ & + e^{-t|k|^2} \frac{\mathcal{F}(Pu_0)(k_1, k_2)}{k_1 k_2}, \end{aligned} \quad (2.3.8)$$

where \tilde{P} denotes the reflection operator $\tilde{P}(f)(r, s) = -2f(r, s) + 2f(-r, s)$.

Proof. The fundamental solution of the heat equation in the two-dimensional quarter space can be computed with the help of the method of reflection. It yields

$$\begin{aligned} u(x, t) = & \int_{\mathbb{R}_+ \times \mathbb{R}_+} \bar{G}(x, y, t) u_0(y) dy + \int_0^t \int_{\mathbb{R}_+} \partial_{y_1} \bar{G}(x, y, t-s) g_1(y_1, s) \Big|_{y_2=0} dy_1 ds \\ & + \int_0^t \int_{\mathbb{R}_+} \partial_{y_2} \bar{G}(x, y, t-s) g_2(y_2, s) \Big|_{y_1=0} dy_2 ds =: u_1(x, t) + u_2(x, t), \end{aligned}$$

where u_1 and u_2 represent the respective influence of the initial and boundary data. $\bar{G}(x, y, t)$ – the Green's function (in the 2D quarterspace) – can be computed explicitly:

$$\bar{G}(x, y, t) = \frac{1}{4\pi t} \left(e^{-\frac{|y-x|^2}{4t}} + e^{-\frac{|y+x|^2}{4t}} - e^{-\frac{|y-\tilde{x}|^2}{4t}} - e^{-\frac{|y+\tilde{x}|^2}{4t}} \right).$$

Here $\tilde{x} = (x_1, -x_2)$, $\bar{x} = (-x_1, x_2)$.

As above, this can be rephrased in terms of the whole space fundamental solution. Extending u_0 by 0, the initial data are, for example, propagated according to

$$u_1(x, t) = \int_{\mathbb{R}^2} \bar{G}(x, y, t) u_0(y) dy = \int_{\mathbb{R}^2} G(x, y, t) P u_0(y) dy,$$

where G is the standard Green's kernel for the heat operator and P is the reflection operator defined above. A similar argument yields the expression for u_2 . Thus,

evaluating at time $t = T$, leads to

$$e^{-Tk^2} \mathcal{F}(Pu_0)(k) = e^{-Tk^2} \left(k_1 \int_0^T e^{k^2 s} \mathcal{F}(\tilde{P}g_2)(k_2, s) ds + k_2 \int_0^T e^{k^2 s} \mathcal{F}(\tilde{P}g_1)(k_1, s) ds \right).$$

Dividing by k_1, k_2 finally implies the claim. \square

With this preparation, we can finally attack the proof of Proposition 4.

Proof of Proposition 4. Again, we strongly rely on the representation formula, (2.3.8). Without loss of generality, we may assume that there exist $k_1, k_2 \in \mathbb{R} \setminus \{0\}$ such that

$$\frac{\mathcal{F}(\tilde{P}g_{11})(k_1)}{k_1} \neq 0 \text{ and } \frac{\mathcal{F}(\tilde{P}g_{21})(k_2)}{k_2} \neq 0,$$

as due to the representation formula, (2.3.8), the situation would otherwise reduce to the one-dimensional case treated in the previous statements, e.g. Proposition 5. In order to prove the claim of the proposition, we distinguish two cases. In the first case, we assume that, asymptotically, the weighted integrals of $g_{12}(s)$ and $g_{22}(s)$ differ. Without loss of generality (and by passing to subsequences which we suppress in our notation), we may assume that

$$\left| \int_0^T e^{|k|^2 s} g_{12}(s) ds \right| > \left| \int_0^T e^{|k|^2 s} g_{22}(s) ds \right|, \quad (2.3.9)$$

as $|k| \rightarrow \infty$. By virtue of the representation formula, (2.3.8), this implies

$$\begin{aligned} \left| \frac{\mathcal{F}u_0(k)}{k_1 k_2} \right| &\geq \left| \int_0^T e^{|k|^2 s} \frac{\mathcal{F}(\tilde{P}g_1)(k_1, s)}{k_1} ds \right| - \left| \int_0^T e^{|k|^2 s} \frac{\mathcal{F}(\tilde{P}g_2)(k_2, s)}{k_2} ds \right| \\ &= \left| \frac{\mathcal{F}(\tilde{P}g_{11})(k_1)}{k_1} \right| \left| \int_0^T e^{|k|^2 s} g_{12}(s) ds \right| - \left| \frac{\mathcal{F}(\tilde{P}g_{21})(k_2)}{k_2} \right| \left| \int_0^T e^{|k|^2 s} g_{22}(s) ds \right|. \end{aligned} \quad (2.3.10)$$

As

- the left hand side of (2.3.10) vanishes in the limit $|k_2| \rightarrow \infty$,
- the assumption (2.3.9) implies that the second term on the right hand side is asymptotically strictly smaller than the first term (along respective subsequences and for an appropriately chosen fixed $k_1 \in \mathbb{R} \setminus \{0\}$),
- $\left| \frac{\mathcal{F}(\tilde{P}g_{21})(k_2)}{k_2} \right| \rightarrow 0$ as $|k_2| \rightarrow \infty$,

Lemma 3 implies $g_{12} \equiv 0$. As a consequence of (2.3.9) and Lemma 3, this also induces $g_{22} \equiv 0$. Thus, $u \equiv 0$.

Hence, we proceed with the second case. Here, we assume that

$$\left| \int_0^T e^{|k|^2 s} g_{12}(s) ds \right| = \left| \int_0^T e^{|k|^2 s} g_{22}(s) ds \right|, \quad (2.3.11)$$

asymptotically. Fixing k_1 such that $\left| \frac{\mathcal{F}\tilde{P}(g_{11})(k_1)}{k_1} \right| \neq 0$, taking the limit $k_2 \rightarrow \infty$ and noting $|\mathcal{F}\tilde{P}(g_{21})(k_2)| \leq C$, this again amounts to an inequality that cannot be satisfied unless $g_{12} \equiv 0$. Hence, $u \equiv 0$. Combining the two cases, yields the full claim. \square

Remark 6. • The argument strongly relies on the product structure of $\mathbb{R}_+ \times \mathbb{R}_+$ and the separation of variables in $g_1(x_1)$ and $g_2(x_2)$. A similar argument for smaller angles (e.g. the case of $\theta = 45^\circ$) fails as this orthogonality property is lost: From a technical point of view, the separation of variables in (2.3.10) does not work any more. This can be interpreted as an indication of the criticality of domains with an opening angle of 90° .

- The argument generalizes to arbitrary dimensions, i.e. domains of the form $\mathbb{R}_+ \times \dots \times \mathbb{R}_+$.

Discussion

We conclude this section with a brief discussion of the limitations of the direct approach. Although the direct approach is very tempting and provides good intuition for the optimal angular dependence, it suffers from several drawbacks:

- Similar to the methods employed by Zuazua and Micu, the presented techniques are restricted to a very narrow class of equations where explicit Green's function control (in Fourier space) is possible.
- Furthermore, it is not clear how to pass from the case of separable boundary data (of Proposition 4) to the general case, as this might entail oscillations which cannot be controlled with the aid of the presented tools.

Therefore, a more abstract approach appears inevitable. This is pursued in the next sections.

2.4 Statement of the Main Results

In this section we present the main results on the backward uniqueness property for the heat equation in two spatial dimensions. These will be derived as consequences of certain Carleman estimates. Using the notation

$$\Omega_\theta = \left\{ (x_1, x_2) \in \mathbb{R}^2 \mid \tan(\theta/2) \geq \frac{|x_2|}{x_1}, x_1 \geq 0 \right\} \subset \mathbb{R}^2,$$

we have:

Proposition 6 (Carleman Estimate). *Let $u \in C_0^\infty([0, T] \times (\Omega_\theta \setminus B_R(0)))$, $R \gg 1$ sufficiently large, $\theta \geq 95^\circ$. Then there exists a Carleman weight $\phi(t, x)$, $|\phi(t, x)| < C\frac{|x|^2}{t}$ such that*

$$\tau \left\| e^{\tau\phi} \frac{(1-t)^{\frac{1}{2}}}{t} u \right\|_{L^2} + \tau^{\frac{1}{2}} \|e^{\tau\phi} u\|_{L^2} + \|e^{\tau\phi} \nabla u\|_{L^2} \lesssim \|e^{\tau\phi} (\partial_t + \Delta) u\|_{L^2}. \quad (2.4.1)$$

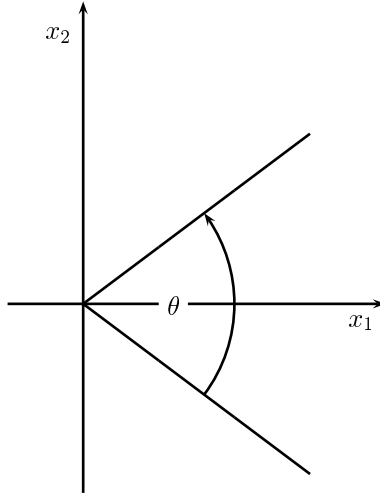


Figure 2.1: The domain Ω_θ .

The difficulty in proving this estimate stems from the loss of convexity of the weight function. Due to the restrictions on its radial growth (which is necessary if the inequality is to be applied to the backward uniqueness problem), it cannot be easily convexified in the radial direction which would simplify the proof of the Carleman inequalities significantly.

As in [LŠ10], the backward uniqueness property is a direct consequence of the Carleman estimate:

Proposition 7 (Backward Uniqueness of the Heat Equation in Angular Domains).

Let $\theta \geq 95^\circ$ and assume that $u : [0, 1] \times \Omega_\theta \rightarrow \mathbb{R}$ satisfies

$$\begin{aligned} |(\partial_t + \Delta)u| &\leq C(|u| + |\nabla u|) \text{ in } [0, 1] \times \Omega_\theta, \\ u(0, x) &= 0 \text{ in } \Omega_\theta, \\ |u| &\leq M \text{ in } [0, 1] \times \Omega_\theta. \end{aligned} \quad (2.4.2)$$

Then $u = 0$.

Remark 7. The angle $\theta \geq 95^\circ$ is not optimal. Various numerical experiments suggest that evaluating the one-dimensional pseudoconvexity condition, i.e. expression (2.6.2), it is possible to reach angles of less than 95° . However, the gain seems to be marginal (one reaches angles of $\sim 94.8^\circ$); in fact, it seems not easy to reach angles of less than 94° (via one-dimensional weight functions).

Under the additional assumption that both the initial and final data vanish, it is possible to prove the backward uniqueness property in angles strictly larger than 90° in two dimensions. This is a nontrivial result depending strongly on the *unboundedness* of the underlying domain. In fact, in any *bounded* domain it would be possible to find a large variety of boundary controls satisfying the initial and final condition.

As in the dissertation of Li [Li11], this (conditional) uniqueness statement is a consequence of decay properties of the underlying *elliptic* problem: In domains of opening angles greater than or equal to 90° there are no harmonic functions decaying with a Gaussian rate. Instead of employing the Phragmen-Lindelöf theorem for harmonic functions (as Li does), we argue via an elliptic Carleman estimate for which we use a limiting Carleman weight in the sense of Kenig et al. [KSU07]. Compared with the Phragmen-Lindelöf-Ansatz this strategy seems to be more stable and allows to include lower order perturbations (with time independent coefficients).

Proposition 8 (Uniqueness of the Control Function in L^2). *Let $\theta > \frac{\pi}{2}$, $\alpha = \frac{\pi}{\theta}$ and assume that $u : [0, 1] \times \Omega_\theta \rightarrow \mathbb{R}$ satisfies*

$$\begin{aligned} (\partial_t + \Delta)u &= c_1(x)u + c_2(x) \cdot \nabla u \text{ in } [0, 1] \times \Omega_\theta, \\ |c_2(x)| &\leq C \frac{1}{|x|^{b(\theta)}} \text{ in } \Omega_\theta, \\ u(1, x) &= 0 \text{ in } \Omega_\theta, \\ u(0, x) &= 0 \text{ in } \Omega_\theta, \\ |u| &\leq M \text{ in } [0, 1] \times \Omega_\theta, \end{aligned} \tag{2.4.3}$$

where $b(\theta) > \frac{2-\alpha}{\alpha}$ and $c_1 \in L^\infty$. Then $u \equiv 0$.

Remark 8. Proposition 8 demonstrates the uniqueness of the possible control function for the heat equation in an unbounded, conical domain of opening angle $\theta > \frac{\pi}{2}$. This is in sharp contrast with the results for the heat equation in bounded domains, in which case there are infinitely many possibilities for such controls [LR95].

Remark 9. Matsaev and Gurarii [GM84] claim that the backward uniqueness result for the pure heat equation can be reduced to an existence result for the Laplacian even if no additional assumption on the behavior of $u(1, x)$ is made. However, there seems to be no proof of this statement in the literature.

2.5 Proofs of the Elliptic Carleman Estimates and Consequences

The Elliptic Pseudoconvexity Analysis

As indicated in Chapter 1 a key step in proving a Carleman estimate consists of the analysis of the conjugated operator. In choosing our weight, we consider a general

ansatz of the form $\tau\phi$ with the aim of proving an inequality of the type (1.0.1) with $P(x, D) = \Delta$. Calculating the conjugated operator yields

$$L_\phi = e^{\tau\phi} \Delta e^{-\tau\phi} = \Delta - 2\tau \nabla\phi \cdot \nabla + \tau^2 |\nabla\phi|^2 - \tau \Delta\phi.$$

The symmetric and antisymmetric parts of this operator are given by

$$\begin{aligned} S_\phi &= \Delta + \tau^2 |\nabla\phi|^2, \\ A_\phi &= -2\tau \nabla\phi \cdot \nabla - \tau \Delta\phi. \end{aligned}$$

We remark that although the original operator was elliptic, the resulting symmetric and antisymmetric parts of the conjugated operator are not elliptic anymore. Expanding the L^2 norm of L_ϕ , we thus infer

$$\|L_\phi w\|_{L^2(\Omega)}^2 = \|S_\phi w\|_{L^2(\Omega)}^2 + \|A_\phi w\|_{L^2(\Omega)}^2 + \int_{\Omega} ([S_\phi, A_\phi]w, w) dx,$$

for $w \in C_0^\infty(\Omega)$. Hence, on the intersections of the characteristic sets of the symmetric and antisymmetric parts, the necessary amount of positivity has to originate from the commutator:

$$\int_{\Omega} ([S_\phi, A_\phi]w, w) dx = \int_{\Omega} 4\tau^3 \nabla\phi \cdot \nabla^2 \phi \nabla\phi w^2 + 4\tau \nabla w \cdot \nabla^2 \phi \nabla w - \tau \Delta^2 \phi w^2 dx.$$

In order to understand the behaviour of this expression, it is helpful to switch to a microlocal point of view. The principal symbols of the symmetric, antisymmetric and commutator part turn into

$$\begin{aligned} p^r &= -|\xi|^2 + \tau^2 |\nabla\phi|^2, \\ p^i &= -2\tau \nabla\phi \cdot \xi, \\ \{p^r, p^i\} &= 4(\tau^3 \nabla\phi \cdot \nabla^2 \phi \nabla\phi + \tau \xi \cdot \nabla^2 \phi \xi). \end{aligned}$$

Therefore, the intersection of the characteristic set of the symmetric and antisymmetric parts of the operator is given by

$$\{|\xi|^2 = \tau^2 |\nabla\phi|^2\} \cap \{\nabla\phi \cdot \xi = 0\}.$$

In the two-dimensional setting this leads to simplifications in the Poisson bracket:

$$\{p^r, p^i\} = 4\tau^3 \Delta\phi |\nabla\phi|^2 \text{ in } \{|\xi|^2 = \tau^2 |\nabla\phi|^2\} \cap \{\nabla\phi \cdot \xi = 0\}.$$

Hence, the corresponding pseudoconvexity condition for the weight turns into subharmonicity:

$$\Delta\phi \geq 0 \text{ in } \{|\xi|^2 = \tau^2 |\nabla\phi|^2\} \cap \{\nabla\phi \cdot \xi = 0\}.$$

In the sequel we will construct weights satisfying this property with sufficient decay in infinity. These are exactly the “limiting Carleman weights” of Kenig et al. [DSFKSU09], [KSU07].

Carleman Inequalities for the Laplacian in Conical Domains

Before turning to the proof of Proposition 8, we first focus on Carleman inequalities for the Laplacian on conical domains. For this purpose, we use weights which are concentrated in the interior of the domain and vanish on the boundary – the necessity of this stems from the lack of control of the boundary and initial data. The explicit choice of the weight is motivated by the requirement of satisfying the elliptic pseudoconvexity condition – which amounts to a considerably easier condition than the corresponding parabolic analogue.

We prove the Carleman estimate by rescaling a local estimate. As the weight which we use satisfies a strict pseudoconvexity condition on $\Omega_\theta \setminus B_1$, the symbol calculus directly implies the estimate

Proposition 9. *Let $\Omega_\theta \subset \mathbb{R}^2$ be the conical domain defined above with $\frac{\pi}{2} < \theta < \pi$. Let $\phi(x, y) = \Re((x + iy)^\alpha) + \epsilon x^\alpha$, with $\alpha = \frac{\pi}{\theta}$, $\epsilon > 0$ arbitrary. Then for $\tau \geq \tau_0 > 0$ it holds*

$$\begin{aligned} \tau^3 \left\| e^{\tau\phi} |x|^{\frac{3\alpha-4}{2}} u \right\|_{L^2(\Omega_\theta \cap (B_2 \setminus B_1))}^2 + \tau \left\| e^{\tau\phi} |x|^{\frac{\alpha-2}{2}} \nabla u \right\|_{L^2(\Omega_\theta \cap (B_2 \setminus B_1))}^2 \\ \lesssim \left\| e^{\tau\phi} \Delta u \right\|_{L^2(\Omega_\theta \cap (B_2 \setminus B_1))}^2 \end{aligned}$$

for all $u \in C_0^\infty(\Omega_\theta \cap (B_2 \setminus B_1))$.

Proof of Proposition 9. This follows immediately from a pseudoconvexity analysis, see for example [Tat96], [Tat99a]. \square

With this and the scaling properties of the weight, the global estimate can be obtained via a decomposition and rescaling procedure.

Proposition 10. *Let $\Omega_\theta \subset \mathbb{R}^2$ be the conical domain defined above with $\frac{\pi}{2} < \theta < \pi$. Let $\phi(x, y) = \Re((x + iy)^\alpha) + \epsilon x^\alpha$, with $\alpha = \frac{\pi}{\theta}$, $\epsilon > 0$ arbitrary. Then for $\tau \geq \tau_0 > 0$ we have*

$$\tau^3 \left\| e^{\tau\phi} |x|^{\frac{3\alpha-4}{2}} u \right\|_{L^2(\Omega_\theta \setminus B_1)}^2 + \tau \left\| e^{\tau\phi} |x|^{\frac{\alpha-2}{2}} \nabla u \right\|_{L^2(\Omega_\theta \setminus B_1)}^2 \lesssim \left\| e^{\tau\phi} \Delta u \right\|_{L^2(\Omega_\theta \setminus B_1)}^2 \quad (2.5.1)$$

for all $u \in C_0^\infty(\Omega_\theta \setminus B_1(0))$.

Proof of Proposition 10. Using a decomposition of space, a scaling argument yields the claim: We decompose $u = \sum_{i \in \mathbb{N}} u_i$, $u_i(x) := (u\eta_i)(x) := u(x)\eta(\frac{|x|-2^i}{2^i})$, where $\text{supp}(\eta) \subset (0.5, 2.5)$, i.e. η is a cut-off function normalized so as to provide a

partition of unity. Setting $v_i(x) := u_i(2^i x)$, we obtain

$$\begin{aligned}
\tau^3 \left\| e^{\tau\phi} |x|^{\frac{3\alpha-4}{2}} u \right\|_{L^2(\Omega_\theta \setminus B_1)}^2 &\lesssim \tau^3 \sum_{i \in \mathbb{N}} \left\| |x|^{\frac{3\alpha-4}{2}} e^{\tau\phi} u_i \right\|_{L^2((\Omega_\theta \cap B_{2^{i+1}}) \setminus B_{2^i})}^2 \\
&= \tau^3 \sum_{i \in \mathbb{N}} \left\| |2^i x|^{\frac{3\alpha-4}{2}} e^{\tau\phi(2^i x)} (\eta u)(2^i x) \right\|_{L^2((\Omega_\theta \cap B_2) \setminus B_1)}^2 2^{in} \\
&\lesssim \sum_{i \in \mathbb{N}} \tilde{\tau}^3 2^{-4i} \left\| e^{\tilde{\tau}\phi(x)} v_i(x) \right\|_{L^2((\Omega_\theta \cap B_2) \setminus B_1)}^2 2^{in} \\
&\stackrel{Prop.9}{\lesssim} \sum_{i \in \mathbb{N}} 2^{-4i} \left\| e^{\tilde{\tau}\phi(x)} \Delta v_i(x) \right\|_{L^2((\Omega_\theta \cap B_2) \setminus B_1)}^2 2^{in} \\
&\lesssim \sum_{i \in \mathbb{N}} \left\| e^{\tau\phi(x)} \Delta u_i(x) \right\|_{L^2((\Omega_\theta \cap B_{2^{i+1}}) \setminus B_{2^i})}^2 \\
&\lesssim \left\| e^{\tau\phi} \Delta u \right\|_{L^2(\Omega_\theta \setminus B_1)}^2 \\
&\quad + \left\| e^{\tau\phi} |x|^{-1} |\nabla u| \right\|_{L^2(\Omega_\theta \setminus B_1)}^2 + \left\| e^{\tau\phi} |x|^{-2} u \right\|_{L^2(\Omega_\theta \setminus B_1)}^2,
\end{aligned}$$

where we used the notation $\tilde{\tau} = 2^{i\alpha} \tau$. In this estimate the last terms are error terms originating from the partition of unity. These will be absorbed in the left hand side for sufficiently large τ .

Analogously, the result for the gradient term can be derived:

$$\begin{aligned}
\tau \left\| e^{\tau\phi} |x|^{\frac{\alpha-2}{2}} \nabla u \right\|_{L^2(\Omega_\theta \setminus B_1)}^2 &\lesssim \tau \sum_{i \in \mathbb{N}} \left\| e^{\tau\phi} |x|^{\frac{\alpha-2}{2}} |\nabla u_i| \right\|_{L^2(\Omega_\theta \cap B_{2^{i+1}} \setminus B_{2^i})}^2 \\
&= \tau \sum_{i \in \mathbb{N}} \left\| e^{\tau\phi(2^i x)} |2^i x|^{\frac{\alpha-2}{2}} |\nabla(u\eta)(2^i x)| \right\|_{L^2((\Omega_\theta \cap B_2) \setminus B_1)}^2 2^{in} \\
&\lesssim \tilde{\tau} \sum_{i \in \mathbb{N}} 2^{-4i} \left\| e^{\tilde{\tau}\phi(x)} |x|^{\frac{\alpha-2}{2}} |\nabla v_i(x)| \right\|_{L^2((\Omega_\theta \cap B_2) \setminus B_1)}^2 2^{in} \\
&\stackrel{Prop.9}{\lesssim} \sum_{i \in \mathbb{N}} 2^{-4i} \left\| e^{\tilde{\tau}\phi(x)} \Delta v_i(x) \right\|_{L^2((\Omega_\theta \cap B_2) \setminus B_1)}^2 2^{in} \\
&\lesssim \sum_{i \in \mathbb{N}} \left\| e^{\tau\phi(x)} \Delta u_i(x) \right\|_{L^2((\Omega_\theta \cap B_{2^{i+1}}) \setminus B_{2^i})}^2 \\
&\lesssim \left\| e^{\tau\phi} \Delta u \right\|_{L^2(\Omega_\theta \setminus B_1)}^2 \\
&\quad + \left\| e^{\tau\phi} |x|^{-1} |\nabla u| \right\|_{L^2(\Omega_\theta \setminus B_1)}^2 + \left\| e^{\tau\phi} |x|^{-2} u \right\|_{L^2(\Omega_\theta \setminus B_1)}^2.
\end{aligned}$$

Adding both inequalities and noting $\frac{3\alpha-4}{2} \geq -2$, $\frac{\alpha-2}{2} \geq -1$ for $\alpha \geq 0$, the error terms can be absorbed. This yields the desired estimate. \square

Proof of Proposition 8 and an Alternative Non-Existence Proof of Harmonic Functions with Gaussian Decay Rates in Cones with Opening Angles Larger than $\frac{\pi}{2}$

In the sequel we assume $\alpha > \frac{4}{3}$, which translates into a condition on the opening angle of the domain: $\theta < \frac{3\pi}{4}$. The backward uniqueness result for conical domains

with larger opening angles immediately follows from this by restriction. It is deduced from the *elliptic* Carleman estimates by an application of the Laplace or a one-sided Fourier transform. Indeed, the t -independence of the coefficients of equation (2.4.3) and Šverák's decay result, Lemma 5, lead to

$$\begin{aligned} s\mathcal{L}u(s, x) + \Delta\mathcal{L}u(s, x) &= c_1(x)\mathcal{L}u(s, x) + c_2(x) \cdot \nabla\mathcal{L}u(s, x) \text{ in } \mathbb{R} \times \Omega_\theta, \\ |\mathcal{L}u| &\leq Ce^{-\beta|x|^2} \text{ in } \mathbb{R} \times \Omega_\theta. \end{aligned}$$

The backward uniqueness result is derived as a consequence of a Carleman estimate – more precisely, of the elliptic estimate (2.5.1). Keeping s fixed and rescaling in x , it is possible to assume the “smallness” condition:

$$\begin{aligned} |\Delta\mathcal{L}u(s, x)| &\leq \lambda(|\tilde{c}_1(x)||\mathcal{L}u(s, x)| + |c_2(x)||\nabla\mathcal{L}u(s, x)|) \text{ in } \mathbb{R} \times \Omega_\theta, \\ |u| &\leq Ce^{-\beta\lambda^2|x|^2} \text{ in } \mathbb{R} \times \Omega_\theta, \end{aligned} \quad (2.5.2)$$

with $\lambda \leq 1$ and $\tilde{c}_1 = c_1 + |s|$. Using (smooth) cut-off functions which satisfy the following limiting behaviour

$$w_{1,R}(x_1) := \begin{cases} 0, & x_1 \leq R, \\ 1, & x_1 \geq 2R, \end{cases} \quad w_2(r) := \begin{cases} 0, & r \leq -\frac{4}{3}, \\ 1, & r \geq -\frac{1}{2}, \end{cases} \quad \eta_L(r) := \begin{cases} 1, & r \leq L, \\ 0, & r \geq 2L, \end{cases}$$

we insert $v_{R,L}(x) := \mathcal{L}u(x)w_{1,R}(x_1)w_2(\phi)\eta_L(|x|)$ into the Carleman inequality (2.5.1). Recalling the decay condition on the function $\mathcal{L}u$ and invoking the dominated convergence theorem, we can pass to the limit $L \rightarrow \infty$. For $v_R := \mathcal{L}uw_{1,R}w_2(\phi)$ we then obtain

$$\begin{aligned} \tau^3 \left\| e^{\tau(\phi-C)} |x|^{\frac{3\alpha-4}{2}} v_R \right\|_{L^2(\Omega_\theta \setminus B_1)}^2 + \tau \left\| e^{\tau(\phi-C)} |x|^{\frac{\alpha-2}{2}} \nabla v_R \right\|_{L^2(\Omega_\theta \setminus B_1)}^2 \\ \lesssim \left\| e^{\tau(\phi-C)} \Delta v_R \right\|_{L^2(\Omega_\theta \setminus B_1)}^2. \end{aligned}$$

Defining $\tilde{w} := w_{1,R}w_2$, we inspect the right hand side of the inequality:

$$\Delta v_R = \tilde{w} \Delta \mathcal{L}u + 2\nabla \tilde{w} \cdot \nabla \mathcal{L}u + \mathcal{L}u \Delta \tilde{w}.$$

Combining this with inequality (2.5.2) and choosing $R \geq 1$ sufficiently large, yields

$$|\Delta v_R| \leq C\lambda(|x|^{\frac{3\alpha-4}{2}}|v_R| + |x|^{\frac{\alpha-2}{2}}|\nabla v_R|) + 2|\nabla \tilde{w}||\nabla \mathcal{L}u| + |\mathcal{L}u||\Delta \tilde{w}|. \quad (2.5.3)$$

Thus, the first term on the right hand side can be absorbed into the left hand side of the Carleman inequality. The remaining right hand side terms in (2.5.3) are only active close to the boundary as well as at a spatial scale $\sim R$. With $R \sim 1$ and choosing $C > 0$ in dependence of R , this leads to a right hand side term of the form

$$\left\| e^{\tau(\phi-C)} (|\nabla \tilde{w}||\nabla \mathcal{L}u| + |\mathcal{L}u||\Delta \tilde{w}|) \right\|_{L^2(\Omega_\theta \setminus B_1)} \lesssim \left\| e^{-\tau\frac{C}{2}} e^{-\beta|x|^2} P_\phi(x) \right\|_{L^2(\Omega_\theta \setminus B_1)},$$

where P_ϕ denotes a function with at most polynomial growth. As a consequence, the right hand side term vanishes in the limit $\tau \rightarrow \infty$. Thus, the function $\mathcal{L}u$ must vanish on some open domain. By unique continuation this therefore implies that $\mathcal{L}u \equiv 0$ in the whole domain. As this holds for all Laplace modes s , we obtain the desired result $\mathcal{L}u \equiv 0$, hence $u \equiv 0$.

Remark 10. The Carleman estimate (2.5.1) dictates the decay assumption on the potential c_2 . Comparing exponents, we obtain

$$b(\theta) = \frac{\alpha - 2}{2}$$

for the exponent in Proposition 8.

As an alternative to the complex analytic argument presented in Section 2.2, we can now present a second, more stable proof of the non-existence of harmonic functions with Gaussian decay rates in cones with opening angles greater than $\frac{\pi}{2}$ via our Carleman inequality (2.5.1):

Proposition 11. *Let $\theta > \frac{\pi}{2}$. Let $u : \Omega_\theta \rightarrow \mathbb{R}$ be a solution of*

$$\begin{aligned} \Delta u &= c_1(x)u + c_2(x) \cdot \nabla u \text{ in } \Omega_\theta, \\ |c_2(x)| &\leq \frac{1}{|x|^{b(\theta)}} \text{ in } \Omega_\theta, \quad c_1 \in L^\infty, \\ |u| &\leq e^{-\beta|x|^2} \text{ in } \Omega_\theta. \end{aligned}$$

Then $u \equiv 0$.

Proof. This follows along the lines of the proof of Proposition 8 (after having carried out the Laplace transform). \square

2.6 The Parabolic Situation – Pseudoconvexity Analysis and Weights for the Anisotropic Operator

The Pseudoconvexity Condition

As we are interested in proving an anisotropic Carleman inequality, we treat the temporal and spatial variables according to the parabolic scaling in the usual conjugation procedure, c.f. [Tat97], [Tat03]. Using an arbitrary weight, ϕ , and setting $u = e^{-\phi}w$, this leads to the following expression

$$\|e^\phi(\Delta + \partial_t)u\|_{L^2}^2 = \|(\Delta + |\nabla\phi|^2 - 2\nabla\phi \cdot \nabla - \Delta\phi + \partial_t - \partial_t\phi)w\|_{L^2}^2.$$

Separation into the symmetric and antisymmetric parts yields

$$\begin{aligned} & \|(\Delta + |\nabla\phi|^2 - 2\nabla\phi \cdot \nabla - \Delta\phi + \partial_t - \partial_t\phi)w\|_{L^2}^2 \\ &= \|(\Delta + |\nabla\phi|^2 - \partial_t\phi)w\|_{L^2}^2 + \|(\partial_t - 2\nabla\phi \cdot \nabla - \Delta\phi)w\|_{L^2}^2 \\ &+ \int ([\Delta + |\nabla\phi|^2 - \partial_t\phi, \partial_t - 2\nabla\phi \cdot \nabla - \Delta\phi]w, w)dx. \end{aligned}$$

Taking the anisotropy of the equation into account (and assuming $\phi \sim \tau$), the principal symbols of these expressions read

$$\begin{aligned} p^r &= -|\xi|^2 + |\nabla\phi|^2, \\ p^i &= s - 2\nabla\phi \cdot \xi, \end{aligned}$$

(in a bounded domain). As for all Carleman inequalities, it suffices to derive the estimate on the characteristic set of the principal symbol. Here, the positivity has to originate from the commutator expression. On the characteristic set the leading order terms of the spatial commutator turn into

$$\{p^r, p^i\}_x = 4\nabla\phi \cdot \nabla^2\phi\nabla\phi + 4|\nabla\phi|^2 \frac{\xi}{|\xi|} \cdot \nabla^2\phi \frac{\xi}{|\xi|},$$

while the temporal commutator is of the following form

$$\{p^r, p^i\}_t = -2\partial_t|\nabla\phi|^2.$$

As we will see in the sequel, both terms play an essential role for our analysis:

- **Decay of Null-Controllable Solutions.** An equilibrium condition for the temporal and spatial commutators allows to deduce Gaussian decay for null-controllable solutions of the heat equation. This was proved by Šverák et al. [EŠŠ03], c.f. Lemma 5, and can also be extended (with appropriately adapted exponents) to higher order diffusion equations. The key idea here is to employ non-convex weights in the x -variable which are *not* weighted by the (large) prefactor τ , combined with convex weights in the temporal variable which are weighted by a factor of τ . Although this implies that the *spatial* commutator does not induce positivity on the intersection of the characteristic sets of the symmetric and antisymmetric parts of the operator, positivity can be obtained from the *temporal* part of the commutator. The uttermost, still controllable amount of non-convexity in the spatial part is determined by an equality of the scaling of the most negative commutator contributions, $\nabla\phi \cdot \nabla^2\phi\nabla\phi$, and the strongest positive commutator contributions, $-\partial_t|\nabla\phi|^2$. Thanks to the strong τ weight in time, the temporal commutator provides enough positivity in this case, c.f. Lemma 5.
- **Backward Uniqueness Property.** The spatial terms dictate the necessary conditions for Carleman weights which can be used in proving the backward

uniqueness property. In order to treat arbitrary boundary terms, we have to truncate the weight function on the respective spatial and temporal boundaries. This, however, implies that the weight must be very small at the boundary, while it has to become very large in the (spatial and temporal) interior of the domain. This is achieved via weights with a factor τ both in their spatial and their temporal components. From this we infer the existence of a spatial regime in which the spatial commutator dominates over the temporal one due to its scaling with τ^3 (the temporal part only scales with τ^2). Therefore, it becomes necessary to study the spatial weight in detail.

We proceed with the analysis of the second observation. For that purpose, we consider weights of the form $\tau\phi$ instead of ϕ . Therefore, a necessary and sufficient condition for the positivity of the commutator on the characteristic set is given by

$$\{p^r, p^i\}_x \geq 4\tau^3 \nabla\phi \cdot \nabla^2\phi \nabla\phi + 4\tau^3 |\nabla\phi|^2 \lambda_{\min}(\nabla^2\phi) \geq 0, \quad (2.6.1)$$

where $\lambda_{\min}(\nabla^2\phi)$ is the smallest eigenvalue of the Hessian $\nabla^2\phi$. As a consequence, the weight function has to be chosen such that this property is satisfied. For convex functions ϕ this is always true. However, in order to prove the Carleman estimate, the weight has to be “small” at the boundary of the domain and “large” in the interior. In fact, our Carleman weight has to satisfy the following conditions:

- 1.) The weight function has to vanish on the boundary of the domain (both spatially and temporally on the time slice on which the function itself is not already vanishing), and has to be strictly positive in the (spatial and temporal) interior of the domain. This can be slightly relaxed by asking for weight functions which are “small” (instead of vanishing) on the boundaries of the domain. As a consequence, the weight function has to be concave in the angular variable φ (at least partially). As the pseudoconvexity condition is strictly weaker than the standard convexity notion, it is still possible to find a non-empty class of weights in domains with sufficiently large opening angles.
- 2.) As observed by Escauriaza, Seregin and Šverák [ESŠ03] null-controllable solutions of the heat equation have Gaussian decay at infinity:

Lemma 5 (Gaussian Decay, [ESŠ03]). *Let $u : [0, T] \times B_R(0) \rightarrow \mathbb{R}$ satisfy*

$$\begin{aligned} |\partial_t u + \Delta u| &\leq c_1 (|\nabla u| + |u|) \text{ in } (0, T) \times B_R(0), \\ u(0, x) &= 0 \text{ in } B_R(0), \\ |u| &< M \text{ in } (0, T) \times B_R(0), \end{aligned}$$

for some constant $c_1 < \infty$. Then there exist constants β, γ , such that for $t \in (0, \gamma)$

$$|u(t, 0)| \leq \frac{c_2}{\min\{1, T\}} M e^{-\beta \frac{R^2}{t}},$$

where $c_2 = c_2(c_1)$, $\gamma = \gamma(c_1, T)$.

Microlocally, the estimate of Escauriaza, Šverák and Seregin uses an equilibrium between a relatively weak, non-convex spatial weight and a very strong, convex temporal weight.

Lemma 5 implies that the growth of admissible Carleman weights is restricted: Any Carleman weight, which is constructed with the aim of proving the backward uniqueness property, has to have a subquadratic growth behaviour in unbounded conical domains.

The Ansatz for the Weight Function: Necessary and Sufficient Conditions

In analogy to the weight function of Šverák and Li [LŠ10], we make the ansatz

$$\phi(r, \varphi) := r^\alpha f(\varphi),$$

for a two-dimensional (spatial) weight function in polar coordinates. In this case the pseudoconvexity condition, (2.6.1), can be rephrased as a homogeneous cubic ordinary differential inequality:

$$\begin{aligned} & (\alpha - 1)\alpha^3 f(\varphi)^3 + \alpha(2\alpha - 1)f(\varphi)f'(\varphi)^2 + f'(\varphi)^2 f''(\varphi) \\ & + \frac{1}{2} (\alpha^2 f(\varphi)^2 + f'(\varphi)^2) (\alpha^2 f(\varphi) + f''(\varphi)) \\ & - \sqrt{(\alpha - 2)^2 \alpha^2 f(\varphi)^2 - 2(\alpha - 2)\alpha f(\varphi)f''(\varphi) + 4(\alpha - 1)^2 f'(\varphi)^2 + f''(\varphi)^2} \geq 0. \end{aligned} \tag{2.6.2}$$

Lemma 5, however, implies a restriction on the possible radial dependence of the weight function: $\alpha \leq 2$. Difficulties in choosing appropriate weights therefore stem from the fact that we cannot convexify the weight in the radial variable in an arbitrarily strong manner.

Šverák's Weight Function and a Modification

In order to analyze possible Carleman weights, we briefly review Šverák's ansatz: The weight function

$$\phi_{Sv}(r, \varphi) = r^\alpha \left(\cos^\alpha(\varphi) - \cos^\alpha\left(\frac{\theta}{2}\right) \right) \tag{2.6.3}$$

satisfies the pseudoconvexity condition as long as the opening angle θ remains large enough: $\theta \geq \arccos(\frac{1}{\sqrt{3}})$. The necessity of this condition can be verified by analytically checking the pseudoconvexity condition at the boundary of the domain. Indeed, Šverák's weight function degenerates at the boundary although it displays robust pseudoconvexity properties in the interior (c.f. Figure 2.2). A limitation of Šverák's weight certainly consists in choosing only a one parameter family of

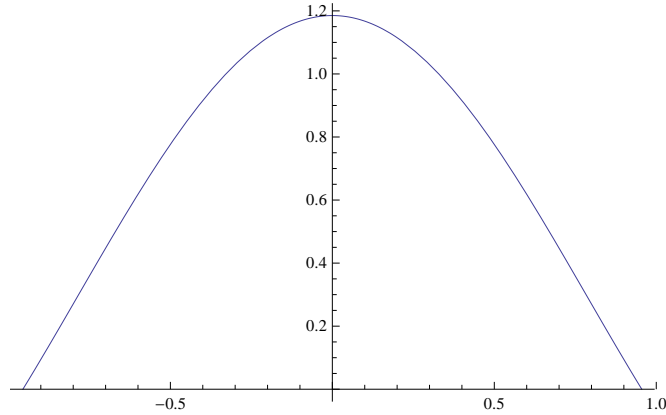


Figure 2.2: The pseudoconvexity condition is satisfied for Šverák's weight function: The x -axis depicts the angle in radians while we plot the values of the pseudoconvexity-expression (2.6.2) on the y -axis. We note that the pseudoconvexity properties of the weight function degenerate at the boundary.

weights. If instead the same weight is considered with a second parameter β , e.g.

$$\phi_{\alpha,\beta}(r, \varphi) = r^\alpha \left(\cos^\beta(\varphi) - \cos^\beta\left(\frac{\theta}{2}\right) \right)$$

the angle can be reduced significantly.

This ansatz has the advantage that although there are restrictions on the growth of α there are none on the size of β , in particular $\beta \geq 2$ is an admissible exponent. Here the weight suffices to prove the backward uniqueness property in opening angles of up to approximately 95.4° . The drawback of this ansatz, however, is that the pseudoconvexity condition can become fragile in the interior of the domain as well (c.f. Fig. 2.3).

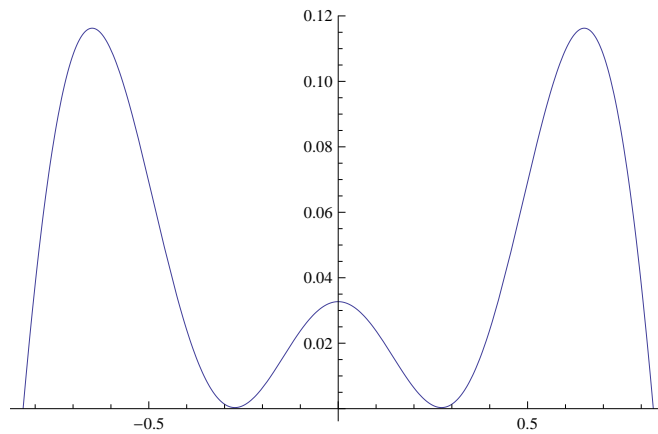


Figure 2.3: For the angle $\theta \sim 95.4^\circ$ the pseudoconvexity condition is satisfied for $\phi_{\alpha,\beta}$ with $\alpha = 1.999999$, $\beta = 2.474917$. For this weight function the pseudoconvexity condition deteriorates at the boundary as well as in the interior.

This two-parameter family of weight functions is certainly not optimal. A more

general ansatz for a weight function could consist of making a power series ansatz and optimizing the coefficients so as to preserve pseudoconvexity in the domain. With the weight

$$\begin{aligned} \phi(r, \varphi) := r^{1.99999} & (0.987609 - 1.22053\varphi^2 + 0.562108\varphi^4 - 0.162117\varphi^6 \\ & + 0.0481833\varphi^8 - 0.000001\varphi^{10}), \end{aligned} \quad (2.6.4)$$

for example, it is possible to reach angles below 95° .

The Numerical Analysis of the Pseudoconvexity Condition

Instead of trying to guess a suitable weight function, it is possible to numerically analyze the pseudoconvexity condition. As the ODE which encodes the one-dimensional pseudoconvexity condition is invariant under the reflection

$$f(\varphi) \mapsto f(-\varphi),$$

we expect the solution to be symmetric if the boundary conditions are prescribed in a symmetric way. Unfortunately, the system seems to be numerically stiff; using Mathematica calculations it seems impossible to reach an angle smaller than approximately 94.8° in the case of an equality in (2.6.2). Therefore, it would be very interesting to understand the symmetric boundary value problem for (2.6.2) from an analytical point of view. Due to the nonlinearity and square root in the equation this seems to be challenging.

Apart from these (technical) difficulties, we believe that the fundamental problem of determining admissible weights via the described one-dimensional approach is limited to approximately 95° . In other words, the major drawback in reaching angles closer to the conjectured 90° is caused by restricting to essentially one-dimensional weight functions.

Proof of the Carleman Estimate (2.4.1)

Using the explicit weight $\phi_{1.999999, 2.474917}$, it is possible to deduce a Carleman inequality and thus to prove backward uniqueness of the heat equation in conical domains with angles down to approximately 95.4° . As the computations for other weights such as (2.6.4) are of a similar flavour but algebraically more complicated, we concentrate on $\phi_{1.999999, 2.474917}$.

Once an admissible, improved weight is found, the techniques of the proof of the backward uniqueness property are not new; in fact we argue along the same lines as Šverák and Li [LŠ10]. As already indicated by the phase space considerations the proof has to use the pseudoconvexity properties of the weight. Although the proof will not be a phase space argument but will instead rely on a direct argument, the previous considerations form the basis of the result. Having ensured pseudoconvexity in the spatial variables, the final weight function can be chosen to have the

following time dependence:

$$\begin{aligned}\phi(t, r, \varphi) &= \phi_1(t, r, \varphi) + \phi_2(t), \\ \phi_1(r, t, \varphi) &= \frac{1-t}{t} \phi_{1.999999, 2.474917}(r, \varphi), \quad \phi_2(t) = \epsilon(1-t)^2,\end{aligned}$$

for a sufficiently small constant $0 < \epsilon \ll 1$ to be chosen later.

Proof of Proposition 6. Let $u \in C_0^\infty((0, T) \times (\Omega_\theta \setminus B_R))$, $R \gg 1$. Conjugating the heat operator gives

$$\begin{aligned}L_\phi u &= (\Delta + \tau^2 |\nabla \phi|^2 - 2\tau \nabla \phi \cdot \nabla - \tau \Delta \phi + \partial_t - \tau \partial_t \phi)u, \\ A_\phi u &= (\partial_t - 2\tau \nabla \phi \cdot \nabla - \tau \Delta \phi)u, \quad S_\phi u = (\Delta + \tau^2 |\nabla \phi|^2 - \tau \partial_t \phi)u.\end{aligned}$$

Therefore the L^2 norm of the operator turns into

$$\int |L_\phi u|^2 dxdt = \int |A_\phi u|^2 dxdt + \int |S_\phi u|^2 dxdt + \int ([S_\phi, A_\phi]u, u) dxdt.$$

The idea is to derive the lower bound by using a combination of the commutator and the symmetric part of the operator. A short calculation yields

$$\begin{aligned}\int ([S_\phi, A_\phi]u, u) dxdt &= 4 \int (\tau^3 \nabla \phi \cdot \nabla^2 \phi \nabla \phi u^2 + \tau \nabla u \cdot \nabla^2 \phi \nabla u) dxdt \\ &\quad + \int (-2\tau^2 \partial_t |\nabla \phi|^2 + \tau \partial_t^2 \phi - \tau \Delta^2 \phi) u^2 dxdt.\end{aligned}$$

As in the case of Šverák and Li [LŠ10], the difficulty originates from the fact that the Hessian of the weight function is not globally positive-definite (which, however, still suffices for our purposes as pseudoconvexity is a strictly weaker condition than the usual notion of convexity). Nevertheless, the numerical analysis of the pseudoconvexity properties of this weight function suggests that on the characteristic set of the symmetric and antisymmetric parts the commutator provides sufficient positivity for the Carleman inequality to hold true. In real space, this condition can be realized by deducing positivity from a combination of the commutator and the symmetric part. As Šverák and Li, we introduce an auxiliary function $F(t, x)$. An integration by parts gives

$$\int (S_\phi u, Fu) dxdt = \int -F |\nabla u|^2 + \left(\frac{1}{2} \Delta F + \tau^2 F |\nabla \phi|^2 - \tau \partial_t \phi F\right) u^2 dxdt.$$

Hence, by the binomial formula

$$\begin{aligned}\int (S_\phi u, S_\phi u) dxdt &\geq - \int (S_\phi u, Fu) dxdt - \frac{1}{4} \int F^2 u^2 dxdt \\ &\geq \int F |\nabla u|^2 - \left(\frac{1}{2} \Delta F + \tau^2 F |\nabla \phi|^2 - \tau \partial_t \phi F\right) u^2 dxdt \\ &\quad - \frac{1}{4} \int F^2 u^2 dxdt.\end{aligned}$$

As in the paper of Šverák and Li [LŠ10], the combination of the commutator and the symmetric part yield

$$\begin{aligned} \int ([S_\phi, A_\phi]u, u) dxdt + \int |S_\phi u|^2 dxdt &\geq \int (4\tau^3 \nabla\phi \cdot \nabla^2\phi \nabla\phi u^2 - \tau^2 F |\nabla\phi|^2 u^2) dxdt \\ &\quad + \int (F |\nabla u|^2 + 4\tau \nabla u \cdot \nabla^2\phi \nabla u) dxdt \\ &\quad + \int (-2\tau^2 \partial_t |\nabla\phi|^2 + \tau \partial_t^2 \phi - \tau \Delta^2 \phi) u^2 dxdt \\ &\quad - \int (\frac{1}{2} \Delta F - \tau \partial_t \phi F) u^2 dxdt - \frac{1}{4} \int F^2 u^2 dxdt. \end{aligned}$$

In order to derive positivity for the gradient term, we set

$$F = -4\tau \lambda_{\min}(\nabla^2 \phi_1) + \frac{2}{5}.$$

We remark that for our choice of ϕ the smallest eigenvalue of the Hessian of ϕ , $\lambda_{\min}(\nabla^2 \phi)$, is a smooth function of both the angular and the radial variables if $r > 0$ (c.f. Figure 2.4). Thus, no additional mollification is necessary in order to deal with expressions as for instance ΔF .

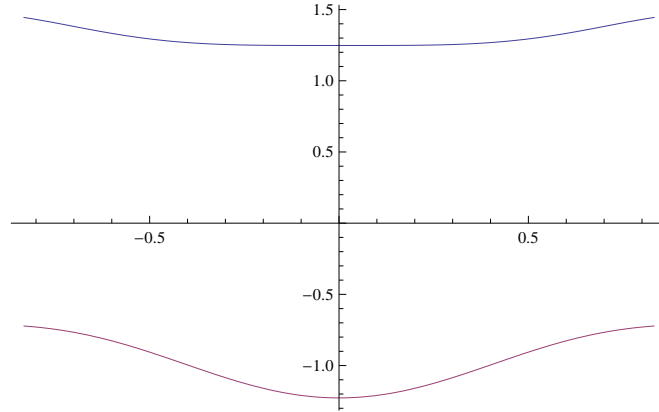


Figure 2.4: The eigenvalues of the Hessian of the weight function ϕ_1 depending on the angular variable φ for fixed radial and temporal variables. Due to the concavity along the angular and the convexity along the radial directions, the eigenvalues have a fixed sign and do not cross. In particular, no mollification is needed in order to deal with the derivatives of the auxiliary function F .

The choice of F immediately implies

$$\int F |\nabla u|^2 + 4\tau \nabla u \cdot \nabla^2 \phi \nabla u dxdt \geq \frac{2}{5} \int |\nabla u|^2 dxdt.$$

As the weight function satisfies the pseudoconvexity condition, we also obtain

$$4\tau^3 \int \nabla\phi \cdot \nabla^2\phi \nabla\phi u^2 + \lambda_{\min}(\nabla^2\phi) |\nabla\phi|^2 u^2 dxdt \geq 0.$$

As a consequence, it remains to prove the positivity of the following terms

$$\begin{aligned} & \int (-2\tau^2 \partial_t |\nabla \phi|^2 + \tau \partial_t^2 \phi - \tau \Delta^2 \phi - \frac{2\tau^2}{5} |\nabla \phi|^2) u^2 dx dt \\ & - \int (\frac{1}{2} \Delta F - \tau \partial_t \phi F) u^2 dx dt - \frac{1}{4} \int F^2 u^2 dx dt. \end{aligned}$$

We begin with the terms of order τ^2 and treat the terms involving ϕ_1 and ϕ_2 separately: We start by estimating the ϕ_1 contributions. Moreover, we note that by choosing $R \gg 1$ sufficiently large, the scaling of $\lambda_{\min}(\nabla^2 \phi)$ in the radial variable implies that the τ^2 contribution coming from the $\frac{1}{4} \int F^2 u^2 dx dt$ integral can be considered small with respect to the other terms of τ^2 scaling. Thus, it will be ignored in the sequel. Due to the homogeneity of the remaining terms in the radial variable ($-2\tau^2 \partial_t |\nabla \phi|^2 - 4\tau^2 \partial_t \phi_1 \lambda_{\min}(\nabla^2 \phi) - \frac{2\tau^2}{5} |\nabla \phi|^2 \sim r^{2\alpha-2}$, $\alpha = 1.999999$) and the multiplicative temporal dependence of the weight, the lower bound

$$\int (-2\tau^2 \partial_t |\nabla \phi|^2 - 4\tau^2 \partial_t \phi_1 \lambda_{\min}(\nabla^2 \phi) - \frac{2\tau^2}{5} |\nabla \phi|^2) u^2 dx dt \geq c\tau^2 \int \frac{(1-t)}{t^2} u^2 dx dt \quad (2.6.5)$$

follows, once it is established in an (angular) cross-section of the domain. In order to deduce this estimate, we observe

$$\begin{aligned} \lambda_{\min}(\nabla^2 \phi) \partial_t \phi_1 &= -\frac{1-t}{t^2} \phi_{\alpha,\beta}(x) \lambda_{\min}(\nabla^2 \phi_{\alpha,\beta}) - \frac{(1-t)^2}{t^3} \phi_{\alpha,\beta} \lambda_{\min}(\nabla^2 \phi_{\alpha,\beta}), \\ \partial_t |\nabla \phi|^2 &= -2\frac{1-t}{t^2} |\nabla \phi_{\alpha,\beta}|^2 - 2\frac{(1-t)^2}{t^3} |\nabla \phi_{\alpha,\beta}|^2, \end{aligned}$$

where $\alpha = 1.9999999$, $\beta = 2.474917$. Thus, it suffices to prove the positivity of

$$3.6 |\nabla \phi_{\alpha,\beta}|^2 + 4\lambda_{\min}(\nabla^2 \phi_{\alpha,\beta}) \phi_{\alpha,\beta}.$$

As this expression attains a positive local minimum at $\varphi = 0$ and as this is a global minimum on our domain of definition, the desired positivity follows, c.f. Fig. 2.5. In order to estimate the full contribution in τ^2 , it remains to bound

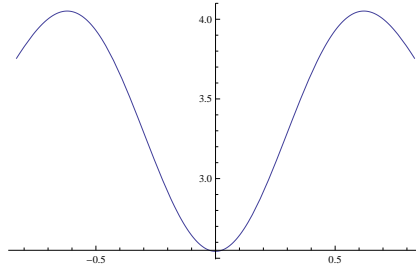


Figure 2.5: The figure depicts the term $3.6 |\nabla \phi_{\alpha,\beta}|^2 + 4\lambda_{\min}(\nabla^2 \phi_{\alpha,\beta}) \phi_{\alpha,\beta}$ with $\alpha = 1.9999999$, $\beta = 2.474917$ in an angular cross-section of the domain. The numerical evaluation shows that this expression is positive.

$$-4\tau^2 \int \partial_t \phi_2 \lambda_{\min}(\nabla^2 \phi) u dx dt = -8\tau^2 \epsilon \int (1-t) \lambda_{\min}(\nabla^2 \phi) u^2 dx dt.$$

For sufficiently small ϵ this can be absorbed into the right hand side of (2.6.5).

We proceed with the terms of τ -scaling. Due to the positivity of $\partial_t^2 \phi_i$, the estimate $|\partial_t^2 \phi_i| \geq |\partial_t \phi_i|$, $i \in \{1, 2\}$, and the scaling in the radial direction, the last term,

$$\tau \int (\partial_t^2 \phi - \Delta^2 \phi - \frac{\tau^{-1}}{2} \Delta F + \frac{2}{5} \partial_t \phi + \frac{2}{5} \lambda_{\min}(\nabla \phi_1)) u^2 dx dt,$$

is positive in the spatial interior of the domain (which in particular includes the time slice $t = 1$) if a sufficiently large ball around the origin is excluded. Close to the spatial boundary the scaling of the involved terms allows to absorb the (potentially) negative parts, i.e.

$$\tau \int (-\Delta^2 \phi - \frac{\tau^{-1}}{2} \Delta F + \frac{2}{5} \lambda_{\min}(\nabla \phi_1)) u^2 dx dt,$$

into (2.6.5) for sufficiently large $\tau \geq \tau_0$ (here it is possible to ignore the also potentially negative contribution $\frac{2}{5} \partial_t \phi$ as it can always be absorbed into the larger positive term $\partial_t^2 \phi$).

Furthermore, a small amount of the $\partial_t^2 \phi_1$ contribution suffices to control the negative $\partial_t \phi_1$ derivative. Hence, we obtain a further positive contribution of the form

$$\tau \int (\partial_t^2 \phi + \frac{2}{5} \partial_t \phi) u^2 dx dt \gtrsim \tau \int u^2 dx dt.$$

For sufficiently large τ , this contribution can then be used to absorb the last negative term: $-\frac{1}{25} \int u^2 dx dt$. \square

Proof of the Backward Uniqueness Result

Due to Lemma 5 null-controllable solutions of the heat equation have exponential decay: For solutions of (2.4.2) the estimate of Šverák, Seregin and Escauriaza yields $|u| \leq C e^{-c \frac{\text{dist}(x, \partial\Omega)^2}{t}}$ – which is, at first sight, only a *non-uniform* decay estimate, deteriorating close to the boundary of the domain. Considering angles strictly larger than 90° , it is possible to reduce the angle slightly while still remaining arbitrarily close to the original angle. In this case Šverák's inequality implies a *uniform* decay estimate:

$$|u| \leq C e^{-c|x|^2}.$$

In order to deduce the backward uniqueness property, we use the following strategy of proof:

- In the first step the angle is reduced slightly, so as to obtain the Gaussian decay estimate globally.
- Secondly, with the aid of a cut-off function, which is active at the boundary

of the domain as well as close to the (spatial) origin, the Carleman estimate can be applied.

- Finally, carrying out the limit $\tau \rightarrow \infty$ provides the desired conclusion.

Proof of Proposition 7. Step 1: Decay estimate, rescaling and choice of the test functions.

We choose $\epsilon > 0$ such that $\delta := \theta - \epsilon \geq \theta_0$ where θ_0 is the angle down to which our Carleman inequalities hold (e.g. $\theta_0 = 95.4^\circ$). Lemma 5 implies Gaussian decay:

$$|u| \leq Ce^{-c\frac{\text{dist}(x, \partial\Omega_\theta)^2}{t}} \leq Ce^{-c\frac{\sin^2(\epsilon/2)|x|^2}{t}}.$$

Due to the assumptions, we have to deal with the differential inequality

$$|(\partial_t + \Delta)u| \leq C(|u| + |\nabla u|).$$

Rescaling u parabolically and translating, i.e.

$$u_\lambda(x, t) := u\left(\lambda^2\left(t - \frac{1}{2}\right), \lambda x\right),$$

we obtain a “small” right hand side:

$$\begin{aligned} |(\partial_t + \Delta)u_\lambda| &\leq C\lambda(|u_\lambda| + |\nabla u_\lambda|) \text{ in } [0, 1] \times \Omega_\delta, \\ u_\lambda(t, x) &= 0 \text{ in } \left(0, \frac{1}{2}\right) \times \Omega_\delta. \end{aligned} \tag{2.6.6}$$

With slight abuse of notation, we will work with u satisfying (2.6.6) in the sequel without changing notation.

In order to apply the Carleman estimate, it is necessary to cut off the solution of the heat equation. Due to this, we introduce the cut-off functions

$$w_{1,R}(x_1) := \begin{cases} 0, & x_1 \leq R, \\ 1, & x_1 \geq 2R, \end{cases} \quad w_2(s) := \begin{cases} 0, & s \leq -\frac{4}{3}, \\ 1, & s \geq -\frac{1}{2}, \end{cases}$$

which are chosen to be smooth interpolations in the intermediate regime. Furthermore, we define

$$\begin{aligned} w(x, t) &:= w_{1,R}(x_1)w_2(\phi(t, x) - C), \\ v(x, t) &:= w(x, t)u(x, t). \end{aligned}$$

Although v does not have compact support, an additional limiting argument combined with the Gaussian decay rate of this function, implies its admissibility in the Carleman estimate.

Step 2: *Application of the parabolic Carleman inequality and limit $\tau \rightarrow \infty$.* An application of the Carleman inequality (2.4.1) leads to

$$\tau^{\frac{1}{2}} \left\| e^{\tau(\phi-C)} v \right\|_{L^2} + \left\| e^{\tau(\phi-C)} \nabla v \right\|_{L^2} \leq \left\| e^{\tau(\phi-C)} (\partial_t + \Delta) v \right\|_{L^2}. \quad (2.6.7)$$

Estimating the right hand side results in

$$|(\partial_t + \Delta)v| \leq C\lambda(|v| + |\nabla v|) + C(|u| + |\nabla u|)(|\partial_t w| + |\nabla w| + |\Delta w|);$$

Due to the smallness of λ , the first part of the expression can be absorbed in the left hand side of (2.6.7). For the remaining part, i.e. $C(|u| + |\nabla u|)(|\partial_t w| + |\nabla w| + |\Delta w|)$, we use the definition of w . Indeed, in the set on which $C(|\partial_t w| + |\nabla w| + |\Delta w|) \neq 0$, we have $\phi - C \leq -\frac{1}{2}$. Consequently,

$$\begin{aligned} & C \left\| e^{\tau(\phi-C)} (|u| + |\nabla u|)(|\partial_t w| + |\nabla w| + |\Delta w|) \right\|_{L^2} \\ & \leq C \left\| e^{-\frac{\tau}{2}} (|u| + |\nabla u|)(|\partial_t w| + |\nabla w| + |\Delta w|) \right\|_{L^2} \\ & \leq C \left\| e^{-\frac{\tau}{2} - \beta|x|^2} P_\phi(x) \right\|_{L^2}, \end{aligned}$$

where $P_\phi(x)$ has at most polynomial growth. In the limit $\tau \rightarrow \infty$ the right hand side of the inequality vanishes. Hence,

$$\tau^{\frac{1}{2}} \left\| e^{\tau(\phi-C)} v \right\|_{L^2} + \left\| e^{\tau(\phi-C)} \nabla v \right\|_{L^2} \leq C \left\| e^{-\frac{\tau}{2}} e^{-\beta|x|^2} P_\phi(x) \right\|_{L^2} \rightarrow 0 \text{ as } \tau \rightarrow \infty.$$

As a result,

$$u = 0 \text{ in } \Omega_\delta \cap \{\phi - C \geq 0\}.$$

Now unique continuation across spatial boundaries implies the desired result. \square

Chapter 3

Unique Continuation for the Fractional Laplacian

3.1 Introduction

In this chapter we encounter another rigidity property – the unique continuation principle. In the last decades, unique continuation has been a very active field of research. In its strong form, it states that if a solution of a certain differential equation vanishes of infinite order at a certain point, it must already vanish globally. This property and its “relative”, the weak unique continuation principle, are of particular interest due to several reasons:

- **Rigidity and Uniqueness.** The unique continuation property is a natural extension of the “identity principle” for harmonic functions: Two harmonic functions which agree up to infinite order at a certain point are identical. As this is a very strong rigidity property of harmonic functions, it is a natural question to ask whether and which other operators possess similar rigidity properties. In particular, it is interesting to investigate up to which extent Schrödinger operators inherit the unique continuation properties (from the Laplacian).
- **Absence of Positive Eigenvalues.** Apart from the intrinsic interest in understanding the rigidity properties of solutions of certain classes of equations, an additional motivation for studying the unique continuation principle is provided by understanding the absence of positive eigenvalues for Schrödinger operators (with potentials). In its simplest form, the absence of positive eigenvalues follows from a theorem of Rellich [Rel43], combined with the weak unique continuation property for Schrödinger operators with bounded potentials. Following the survey article of Kenig [Ken89], we briefly sketch the argument relating the spectral properties of Schrödinger operators, $P(D, x) = -\Delta + V$, to a (weak) unique continuation result:
Assume that V is a compactly supported potential, supported, say, on $B_R(0)$.

Suppose a positive eigenvalue E associated to an L^2 eigenfunction existed. Then Rellich's theorem states that $u \equiv 0$ on $\mathbb{R}^n \setminus B_R(0)$, i.e. the eigenfunction is compactly supported. If the operator

$$-\Delta + V - E$$

has the weak unique continuation property, this implies that $u \equiv 0$ on \mathbb{R}^n . Hence, there can be no positive eigenvalue.

In general, it is of interest for which kind of potentials such a statement holds. Here, the limiting behaviour of the potential, both in compact sets and at infinity, plays a decisive role. For example, in quantum mechanical applications a naturally encountered potential consists of the Coulomb potential which is singular at the origin but also displays long range effects. In order to deal with this and similar situations, it is necessary to investigate unique continuation properties under L^p integrability assumptions for the potential.

More elaborate arguments – and in a sense optimal ones – for the non-existence of positive eigenvalues for Schrödinger operators can, for example, be found in the papers of Jerison & Ionescu [IJ03] and Koch & Tataru [KT06]. In particular, the support condition on the potential can be dropped and replaced by appropriate growth bounds at infinity.

- **Connection to (Nonlinear) Elliptic Problems.** Unique continuation statements can be used to deduce uniqueness of solutions to linear and nonlinear problems. This is similar to the reduction of the uniqueness of certain solutions of the Navier-Stokes equations to the backward uniqueness property of the heat equation, which was mentioned in the previous chapter. A recent example in which strong unique continuation results were used to deduce uniqueness of radial solutions of certain nonlinear equations is, for instance, contained in the article of Frank, Lenzmann and Silvestre [FLS13].

By now, an extensive literature on unique continuation properties has been developed. However, instead of reviewing all of these contributions, we focus on the local model case, i.e. the standard Laplacian, and the non-local family of fractional Laplacian operators with $s \in (0, 1)$. Considering the fractional Laplacian instead of the standard Laplacian is a natural extension as many models describing physical, economic or geometric situations are based on this non-local operator rather than on the local analogues, e.g. [BS02], [Váz12], [CG11], [SV09]. Examples from physics are relativistic Schrödinger equations involving the half-Laplacian or certain approximations of the Navier-Stokes equations [Sil07]. An example originating from economics are so-called American options [Sil10].

In the context of unique continuation properties this non-local, elliptic pseudodifferential operator poses an interesting challenge, as one has to find appropriate means of exploiting the local information, i.e. the local high order of vanishing. More precisely, in the sequel we will consider the following problem: Let $u : \mathbb{R}^n \rightarrow \mathbb{R}$,

$u \in H^s$, $s \in (0, 1)$, be a (weak) solution of

$$(-\Delta)^s u = Vu,$$

where u vanishes of infinite order at a certain point x_0 (which we choose to be 0 in the sequel). Does this already imply that u vanishes identically?

Here, the infinite order of vanishing means that for any $n \in \mathbb{N}$ we have

$$\lim_{r \rightarrow 0} r^{-n} \int_{B_r(0)} u^2 dx = 0.$$

In order to tackle this problem, we crucially rely on the Caffarelli-Silvestre extension. This allows to interpret the fractional Laplacian as a (generalized) Dirichlet-to-Neumann map of a certain degenerate elliptic operator. As a result, the problem becomes tractable via Carleman inequality techniques.

The remaining part of the chapter is organized as follows: In the following two sections we briefly review the literature on unique continuation properties for (standard) Schrödinger equations and recall important properties of the fractional Laplacian. Section 3.4 is dedicated to the statement of the central Carleman estimates. In Sections 3.5-3.7 we prove the decisive Carleman estimate and show how it implies the strong unique continuation principle if $s \in [\frac{1}{4}, 1)$. Here, the methods of deducing the estimates strongly rely on the ideas of [KT01a]. If $s < \frac{1}{4}$, we prove the strong unique continuation property under differentiability conditions on the potential. For this we use a slightly modified strategy of proving the crucial Carleman inequality, c.f. Section 3.6.2. Moreover, we study the one-dimensional situation in detail, as one can hope for stronger results in this case, c.f. Section 3.8. Last but not least, Sections 3.9 and 3.10 deal with generalizations of our main estimates: In Section 3.9 we reduce the integrability assumptions in the case of the half-Laplacian, whereas Section 3.10 is dedicated to the discussion of variable coefficient operators.

3.2 Review: Unique Continuation and Carleman Estimates

Previous Works on Unique Continuation for Second Order Elliptic Operators – Results

As unique continuation properties play an important role in understanding the underlying (elliptic) operator, there has been a huge effort to obtain the strongest possible conditions on the respective metrics and potentials in order to secure unique continuation. Here one has to distinguish between the strong and the weak unique continuation properties:

- The *weak* unique continuation property (WUCP) deals with the question of whether vanishing in an *open* set already leads to global vanishing for solutions

of a given PDE.

- The *strong* unique continuation property (SUCP) is concerned with the problem of whether vanishing of *infinite order* at a point already implies global vanishing for solutions of a given PDE.

As far as (divergence form) perturbations of Schrödinger equations are concerned, the picture is quite complete by now. As this serves as our model case, we briefly review the positive and negative results for the equation

$$\Delta u = Vu + W \cdot \nabla u.$$

- **Heuristics.** In order to understand in which settings unique continuation might hold, it is instructive to consider the case of a high but finite (polynomial) order of vanishing (c.f. [Wol93]): Assuming that $u \in C_0^\infty(B_1(0))$, $u \sim r^k$ for $r \ll 1$, $k \gg 1$, we would expect $\Delta u \sim r^{k-2}$. This implies that $\frac{|\Delta u|}{|u|} \sim r^{-2}$, which just fails to be in $L^{\frac{n}{2}}(B_r(0))$ (where n denotes the space dimension). As a consequence, one expects that potentials V , lying in spaces of $L^{\frac{n}{2}}$ -scaling, are the critical ones for unique continuation. An analogous argument suggests that for gradient potentials, W , the scaling invariant (critical) space is given by $L^n(B_r(0))$.
- **The Potential V .** Considering functions of the form $u = e^{-|\ln(|x|)|^{1+\epsilon}}$, one finds that, in general, the strong unique continuation property does not hold for potentials V in L^p -spaces with $p < \frac{n}{2}$. As a complementary result, the seminal paper of Jerison & Kenig [JK85] demonstrated that it is possible to reach all Sobolev potentials with critical scaling by proving the estimate

$$\| |x|^{-\tau} u \|_{L^p} \lesssim \| |x|^{-\tau} \Delta u \|_{L^{p'}},$$

where $\frac{1}{p'} - \frac{2}{n} = \frac{1}{p}$ and $u \in C_0^\infty(\mathbb{R}^n \setminus \{0\})$. Moreover, an appendix of Stein [Ste85] illustrated that even potentials in certain scaling-critical Lorentz spaces can be controlled under an additional smallness assumption. More precisely, Stein showed that the unique continuation property holds for potentials in $L_w^{\frac{n}{2}}$ with small norms. The necessity of this smallness was later demonstrated by Wolff [Wol92a].

Considering only radial potentials, much more can be said [PW98]. Indeed, unique continuation properties hold in all scale-invariant spaces, i.e. up to L_w^n (with arbitrarily large norms). Further results by Pan [Pan92] and Pan & Wolff [PW98], imply the strong unique continuation property for inequalities of the form

$$|\Delta u| \leq \frac{C}{|x|^2} |u|.$$

This illustrates that the situation is more subtle than pure scaling arguments suggest.

- **The Gradient Potential W .** The investigation of the unique continuation property for equations with *gradient* potentials, turned out to impose substantial additional difficulties. In fact, it became clear that the techniques which yielded the results for the potential V alone were not strong enough to prove the conjectured sharp scaling result. The missing ingredient was found by Wolff who introduced an osculation argument [Wol92b]. The “right” combination of the osculation method and the previously existing techniques, however, was first used in its full power by Koch & Tataru [KT01a]. Here they showed that it is possible to prove unique continuation with $W \in l_w^1(L^n)$ with small norm (the space $l_w^1(L^n)$ consists of functions whose L^n norms are l_w^1 “summable” on dyadic annuli). This result is essentially sharp as one can infer from the counterexamples of Koch & Tataru [KT02] and Wolff [Wol94]. Similar to the case of the potentials V , Pan & Wolff [PW98] prove that one can deal with singular potentials satisfying

$$|\Delta u| \leq \frac{C}{|x|^2}|u| + \frac{\epsilon}{|x|}|\nabla u|,$$

for a sufficiently small constant $\epsilon > 0$. Again, this result is essentially sharp, as it is possible to construct counterexamples for the unique continuation property satisfying the differential inequality

$$|\Delta u| \leq \frac{C}{|x|}|\nabla u|,$$

if $C > 0$ is sufficiently large, c.f. [Wol93].

- **Weak Unique Continuation.** The strongest positive results on weak unique continuation are due to Wolff [Wol93]. He deduces the weak unique continuation property for potentials $V \in L^{\frac{n}{2}}$, $W \in L^n$. On the negative side there are several counterexamples, c.f. [KT02], [KN00], [Man02]. The strongest ones complement the positive results by, for example, showing that for $n \geq 3$ Schrödinger operators with potentials of the form $V \in L^{\frac{n}{2}}$ or $W \in L_w^n$, in general, do not have the unique continuation property.
- **Boundary Unique Continuation.** A question related to unique continuation problems consists of asking whether it is possible to control a Schrödinger equation from the boundary. More precisely, one deals with the question whether the vanishing of u on a relatively open subset V of the boundary of a domain $\Omega \subset \mathbb{R}^n$ and the vanishing of ∇u on a set $\tilde{V} \subset V$ with positive \mathcal{H}^{n-1} measure already implies the global vanishing of u . In dimensions $n \geq 3$ this cannot be relaxed to only requiring that u and ∇u vanish on a common boundary subset of positive \mathcal{H}^{n-1} measure, c.f. [BW90]. For further details we refer to Isakov’s book [Isa06] and the references therein.

In a sense, all the previously mentioned results rely on a spectral gap property of the (spherical) Laplacian (which can be obtained by the explicit knowledge of the eigenfunctions and eigenvalues). The spectral gap condition poses a severe restriction on a given operator. As a consequence, it seems unlikely that this property holds for the operator associated with the fractional Laplacian in the respective conformal coordinates in any dimension larger than one (it could however be that this property holds on very specific manifolds).

In spite of this, in general the results on the standard Laplacian can be considered as a guideline for the setting involving the fractional Laplacian. However, in using the Caffarelli-Silvestre extension strategy, one notices a crucial difference: For the fractional Laplacian the standard potential V , i.e. the equation with

$$(-\Delta)^s u = Vu,$$

poses similar difficulties as the *gradient* potential in the case of the standard Laplacian.

Previous Works on Unique Continuation for Second Order Elliptic Operators – Methods

Essentially two techniques are available in order to prove unique continuation results. On the one hand, there is a huge literature on Carleman estimates including, for example [Hör07], [Isa06], [Isa04], [Kli92], [Tat97]. On the other hand, variational approaches using frequency functions are also often applicable, c.f. [GL86], [GL87], [Lin91], [Lin90], [Ken89]. Both methods rely on underlying (pseudo-)convexity properties of the respective operator. In the sequel, we briefly introduce both methods.

- **Carleman Estimates.** Carleman estimates originate from the study of uniqueness in elliptic Cauchy problems. They were first introduced in Carleman’s fundamental paper of 1939 [Car39]. Here, he used strongly weighted estimates in order to derive uniqueness for a two-dimensional Cauchy problem. Later, the concept of exponentially weighted estimates was further developed by Hörmander who pointed out that the underlying principle of such an estimate consists of a certain convexity notion (which is related to convexity notions in complex analysis). Today, Carleman estimates are an indispensable tool in dealing with a wide range of inverse problem (c.f. [Isa06] and the references therein). A brief outline of the general strategy involved in proving a Carleman estimate was pointed out in the introduction to this part of the thesis, c.f. Chapter 1.
- **The Frequency Function Approach.** In [AJ79] Almgren introduced the notion of a “frequency function” in order to measure the local growth of (harmonic) functions. Garofalo and Lin [GL87] exploited its variational structure in deriving monotonicity properties. These lead to doubling estimates

for the functions under consideration which then imply unique continuation. Similarly to Carleman estimates, frequency function approaches rely on convexity/monotonicity properties. We briefly indicate the main ideas of the frequency function approach: For the Laplacian, one defines

$$D(r) := \int_{B_r} |\nabla u|^2 dx, \quad H(r) = \int_{\partial B_r} u^2 d\mathcal{H}^{n-1}(x), \quad N(r) = \frac{rD(r)}{H(r)}.$$

We observe that the scaling behaviour of $rD(r)$ and $H(r)$ agrees. For eigenfunctions of the Laplacian such as $u(x) = \sin(kx)$, a suitable version of the frequency function $N(r)$ describes the oscillatory behaviour of the associated eigenfunction (one needs to carry out a “harmonic extension” by defining the eigenfunction on an appropriate cone, c.f. the survey article of Zelditch [Zel09] and the references therein). In general, the frequency function encodes the local growth of a function u . For a harmonic function, u , it can be shown that the frequency function is monotone: $N'(r) > 0$. Together with the identity

$$\partial_r \left(\ln \frac{H(r)}{r^{n-1}} \right) = 2 \frac{N(r)}{r},$$

this yields the key doubling estimate:

$$\int_{B_{2r}} u^2 dx \lesssim 2^{-2N(r)} \int_{B_r} u^2 dx.$$

From this it is possible to derive unique continuation properties.

Recently this approach has been used in order to obtain unique continuation properties for the fractional Laplacian [FF13].

3.3 Review: The Fractional Laplacian and the Unique Continuation Property

Various Definitions of the Fractional Laplacian

The fractional Laplacian can be defined in several ways. The most common definitions include the interpretation as a pseudodifferential operator with the aid of the Fourier transform and its definition as a singular integral operator. Further possibilities are given via (generalized) Dirichlet-to-Neumann operators or as generators of certain Lévy processes. These definitions are presented in various papers and books including Caffarelli & Silvestre [CS07], DiNezza & Palatucci & Valdinoci [DNPV11], Cabré & Sire [CS13], Landkof [LD72], Stein [Ste70] and many more. In the sequel we briefly recall the different possibilities.

Interpretation as Singular Integral Operator

It is possible to define the fractional Laplacian as a singular integral: Let $s \in (0, 1)$ and $u \in \mathcal{S}(\mathbb{R}^n)$, then

$$\begin{aligned} (-\Delta)^s u(x) &:= C(n, s) P.V. \int_{\mathbb{R}^n} \frac{u(x) - u(y)}{|x - y|^{n+2s}} dy \\ &= -\frac{C(n, s)}{2} \int_{\mathbb{R}^n} \frac{u(x+y) + u(x-y) - 2u(x)}{|y|^{n+2s}} dy, \end{aligned}$$

where $C(n, s) = \pi^{-\frac{n}{2}} 2^{2s} \frac{\Gamma(\frac{n+2s}{2})}{\Gamma(2-s)} s(1-s)$ is chosen such that the Fourier and singular integral definitions of the fractional Laplacian coincide, c.f. [DNPV11], [CS13]. Duality arguments allow to extend this definition to a much larger class of distributions.

Furthermore, it is possible to define a weak notion of the fractional Laplacian via its Dirichlet form. For $u, v \in \mathcal{S}$ it is given by

$$(u, v)_s = \frac{C(n, s)}{2} \int_{\mathbb{R}^{2n}} \frac{(u(x) - u(y))(v(x) - v(y))}{|x - y|^{n+2s}} dx dy = \int_{\mathbb{R}^n} |\xi|^{2s} \overline{\mathcal{F}u} \mathcal{F}v d\xi.$$

Due to Herbst's inequality [Her77], this defines a scalar product on functions in H^s . This definition of the fractional Laplacian motivates the notion of the associated (homogeneous) fractional Sobolev spaces

$$\|u\|_{\dot{W}^{s,p}}^p := \int_{\Omega} \int_{\Omega} \frac{|u(x) - u(y)|^p}{|x - y|^{n+sp}} dx dy.$$

These can also be interpreted as interpolation spaces between the standard Sobolev spaces.

The solution operator associated with the fractional Laplacian is given by the Riesz kernel, c.f. [LD72]:

$$(-\Delta)^{-s} f(x) = \tilde{C}(n, s)^{-1} \int_{\mathbb{R}^n} \frac{f(y)}{|x - y|^{n-2s}} dy,$$

where $\tilde{C}(n, s) = \pi^{\frac{n}{2}} 2^{2s} \frac{\Gamma(s)}{\Gamma(\frac{n-2s}{2})}$.

Interpretation as a Pseudodifferential Operator via the Fourier Transform

Working in \mathbb{R}^n , it is convenient to define the fractional Laplacian via its Fourier symbol: Let $u \in \mathcal{S}$, then

$$(-\Delta)^s u = \mathcal{F}^{-1}(|\cdot|^{2s} \mathcal{F}u).$$

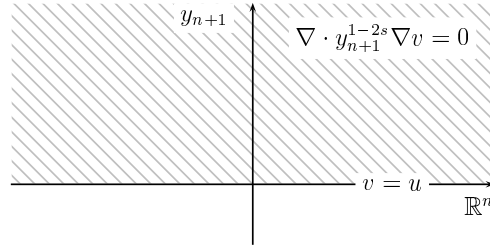


Figure 3.1: The “s-harmonic” extension problem in the upper half-plane.

This notion is not straightforward to handle if one intends to deal with local properties of solutions in real space. However, it is very convenient to obtain (global) properties in Fourier space.

Just as the singular integral definition leads to a certain notion of fractional Sobolev spaces the pseudodifferential notion does as well. This results in the $H^{s,p}$ spaces which are equivalent to the previously mentioned $W^{s,p}$ spaces only if $p = 2$, c.f. [AF03].

Interpretation as Dirichlet-to-Neumann Operator of Certain Degenerate Elliptic Operators

In their celebrated paper [CS07], Caffarelli and Silvestre generalize the interpretation of the half-Laplacian as the Dirichlet-to-Neumann map of the harmonic extension to fractional Laplacian operators with $s \in (0, 1)$. Let v be the “s-harmonic” extension of $u \in \mathcal{S}(\mathbb{R}^n)$, i.e.

$$\begin{aligned} \nabla \cdot y_{n+1}^{1-2s} \nabla v &= 0 \text{ in } \mathbb{R}_+^{n+1}, \\ v &= u \text{ on } \{y_{n+1} = 0\}. \end{aligned}$$

Then, the fractional Laplacian reads

$$(-\Delta)^s u = -c_s \lim_{y_{n+1} \rightarrow 0} y_{n+1}^{1-2s} \partial_{n+1} v.$$

In other words, the fractional Laplacian can be interpreted as a (generalized) Dirichlet-to-Neumann map. The constant c_s does not depend on the dimension n and is given by $c_s = 2^{2s-1} \frac{\Gamma(s)}{\Gamma(1-s)}$ [CS13]. By a slight abuse of notation we will often drop the constant c_s in the sequel.

Although the “s-harmonic” extension is not given by a *uniformly* elliptic equation, the representation as the Dirichlet-to-Neumann map of a *degenerate* elliptic equation allows to use a large machinery in order to obtain existence, uniqueness and regularity properties. In particular, the results on operators in Muckenhoupt classes apply, c.f. [FKS82], [FJK83], [Gra08]. Via duality, it is possible to extend this definition of the fractional Laplacian to a large class of distributions.

Interpretation as a Generator of an α -stable Lévy Process

Finally, a stochastic interpretation is available as well, c.f. [BGR61]. The fractional Laplacian can be interpreted as the infinitesimal generator of an α -stable Lévy process – just as the Laplacian is the generator of Brownian motion. We will not employ this notion in the sequel.

Unique Continuation for the Fractional Laplacian and Previous Results

Recently, the unique continuation problem for the fractional Laplacian has been an area of intense research – just as the whole field of non-local equations, c.f. for example Seo [Seo13a], [Seo13b], Fall & Felli [FF13], Bellová [Bel12], Frank & Lenzmann & Silvestre [FLS13]. We briefly review the most important contributions:

- In terms of the strong unique continuation property the strongest results are given by Fall and Felli [FF13]. The authors prove that for (regular, lower order) perturbations of certain Hardy potentials the strong unique continuation property holds. More precisely, they show that weak solutions of

$$(-\Delta)^s u(x) - \frac{\lambda}{|x|^{2s}} u(x) = h(x)u(x) + f(x, u(x)) \text{ in } \Omega \subset \mathbb{R}^n,$$

satisfy the strong unique continuation principle (at $x = 0$) if

- (a) $n > 2s$, $s \in (0, 1)$, $\lambda < 2^{2s} \frac{\Gamma^2(\frac{n+2s}{4})}{\Gamma^2(\frac{n-2s}{4})}$,
- (b) $h \in C^1(\Omega \setminus \{0\})$, $|h(x)| + |x \cdot \nabla h(x)| \lesssim |x|^{-2s+\epsilon}$, $\epsilon > 0$,
- (c) $f \in C^1(\Omega \times \mathbb{R})$, $t \mapsto F(x, t) \in C^1(\Omega \times \mathbb{R})$ and $|f(x, t)t| + |\partial_t f(x, t)t^2| + |\nabla_x F(x, t) \cdot x| \lesssim |t|^p$ for a.e. $x \in \Omega$ and all $t \in \mathbb{R}$, where $2 < p \leq \frac{2n}{n-2s}$,
 $F(x, t) = \int_0^t f(x, r) dr$.

The proof strongly relies on the Caffarelli-Silvestre extension in order to define an adapted notion of frequency function. For this frequency function, the authors show that the limit $r \rightarrow 0$ exists. In contrast to the usual frequency function arguments, Fall and Felli do not prove monotonicity (of the frequency function). Instead, the existence of the limit $r \rightarrow 0$ suffices in order to argue via a blow-up method, derive an eigenvalue problem and show that this implies the strong unique continuation result.

- In [Seo13a] Seo deals with the weak unique continuation problem by expanding the convolution kernel associated with the fractional Laplacian. In the range $2s \in [n - 1, n)$ the Taylor bounds suffice to derive Carleman-type estimates. This is inspired by the work of Sawyer on the standard Laplacian [Saw84]. Very recently, Seo [Seo13b] improved these estimates by proving a stronger Carleman inequality which is motivated by the estimates in the article of Kenig and Jerison [JK85]. As a result, he obtains the weak unique continuation

principle in the scaling-critical spaces. In fact, he proves the weak unique continuation property for solutions of

$$|(-\Delta)^s u| \leq |Vu| \text{ in } \mathbb{R}^n, \quad n \geq 2,$$

under the assumptions

- (a) $V \in L^{\frac{n}{2s}}_{w,loc}$ with a sufficiently small norm,
- (b) $u \in L^1 \cap L^{p,q}$ and $(-\Delta)^s u \in L^q$ with $p = \frac{2n}{n-2s}$, $q = \frac{2n}{n+2s}$.

if $n \geq 3$, $0 < s < \frac{n}{2}$ and under the assumptions

- (a') $V \in L^p$, $p > \frac{1}{s}$ (more generally, it is possible to work in the Kato class \mathcal{K}_{2s}),
- (b') $u \in L^1$ and $(-\Delta)^s u \in L^1$,

if $n = 2$, $\frac{1}{2} \leq s < 1$.

- Frank & Lenzmann & Silvestre [FLS13] deal with an issue related to unique continuation. They prove that the only radial solution of

$$(-\Delta)^s u = Vu,$$

satisfying the constraints $u(0) = 0$ and $\lim_{r \rightarrow \infty} u(r) = 0$ is the trivial solution, $u \equiv 0$. This allows to deduce uniqueness of ground states for certain nonlinear fractional equations. The authors argue via a monotonicity identity for the “ s -harmonic” extension of the fractional Laplacian.

- Bellová [Bel12] treats the Steklov eigenvalue problem on compact manifolds in her thesis. This can be interpreted as the case $s = \frac{1}{2}$ in our range of fractional exponents. She applies frequency function methods in order to derive doubling inequalities. With these she estimates the Hausdorff-dimension of the nodal lines in the spirit of Yau’s conjecture and derives polynomial bounds.

3.4 The Main Results

We consider the strong unique continuation problem (SUCP) for (weak solutions of) the fractional Laplacian, i.e. $u \in H^s$, $s \in (0, 1)$, satisfies

$$(-\Delta)^s u = Vu \text{ in } \mathbb{R}^n,$$

and vanishes of infinite order at the origin. We prove that under appropriate conditions on V (including scaling-critical Hardy potentials) the solution u vanishes identically:

Proposition 12 (SUCP). *Let $u \in H^s$, $s \in (0, 1)$, solve*

$$(-\Delta)^s u = Vu \text{ in } \mathbb{R}^n, \quad (3.4.1)$$

with $V = V_1 + V_2$,

$$V_1(y) = |y|^{-2s} h \left(\frac{y}{|y|} \right), \quad h \in L^\infty, \quad |V_2(y)| \leq c|y|^{-2s+\epsilon}.$$

For $s < \frac{1}{2}$, we additionally require that one of the following assumptions is satisfied:

- the potential V_2 satisfies $V_2 \in C^1(\mathbb{R}^n \setminus \{0\})$ and $|y \cdot \nabla V_2| \lesssim c|y|^{-2s+\epsilon}$,
- $s \in [\frac{1}{4}, \frac{1}{2})$ and $V_1 \equiv 0$.

Then if u vanishes of infinite order at $y = 0$, this already implies $u \equiv 0$.

Here the infinite order of vanishing is adapted to the degenerate elliptic equation derived via the Caffarelli extension. We define the notions of vanishing of infinite order for bulk and for corresponding boundary integrals.

Definition 5 (Vanishing of Infinite Order). *A function $u \in L^2_{loc}(y_{n+1}^{1-2s} dy, \mathbb{R}^{n+1})$ vanishes of infinite order at zero (in the bulk) if for every $m \in \mathbb{N}$*

$$\lim_{r \rightarrow 0} r^{-m} \int_{B_r^+(0)} y_{n+1}^{1-2s} u^2 dy = 0.$$

A function $u \in L^2_{loc}(\mathbb{R}^n)$ vanishes of infinite order at zero (at the boundary) if for every $m \in \mathbb{N}$

$$\lim_{r \rightarrow 0} r^{-m} \int_{B_r(0)} u^2 dy = 0.$$

In the present work, we approach the problem via Carleman inequalities. We argue in two main steps:

- *Carleman Estimates.* This part constitutes the key estimate: We prove a Carleman inequality at the boundary of the upper half-plane. Our strategy of proving the decisive Carleman estimate relies on methods of Koch and Tataru [KT01a]. We separate the conjugated operator into a radial and a spherical part. Then, we decompose the spherical operator into its eigenspaces. Thus, the necessary estimate is reduced to a bound on (the kernel of) an ordinary differential operator. This procedure allows to handle very rough potentials for $s \geq \frac{1}{4}$ (including scale-invariant ones if $s \geq \frac{1}{2}$). If $s \in (0, \frac{1}{4})$ (and also if $s \in [\frac{1}{4}, \frac{1}{2})$ and involves scaling-invariant potentials), we argue with the help of a slightly modified Carleman estimate which allows to exploit the differentiability assumptions (and regularity properties of solutions to the associated degenerate elliptic equations) in order to deduce the unique continuation property (c.f. Section 3.6.2).

In the case of a sufficiently strong spectral gap, e.g. as in the one-dimensional situation, the unique continuation property can be deduced for any potential which is bounded by a Hardy type potential, $|V(y)| \leq c|y|^{-2s}$ (c.f. Section 3.8) if $s > \frac{1}{2}$ (for $s = \frac{1}{2}$ an additional smallness condition has to be satisfied: $0 < c \ll 1$).

- *Blow-up Procedure.* With the previously discussed preparation, it becomes possible to conclude that if the Caffarelli extension vanishes of infinite order in the tangential and normal directions (with respect to the boundary), it must already vanish identically. Hence, we can concentrate on extensions which only vanish of finite order in the normal direction. For these we consider a blow-up procedure which reduces the problem to the weak unique continuation property.

Our approach does not only complement the article of Fall and Felli [FF13] by relying on Carleman instead of frequency function methods. It also improves their results in three main aspects:

- In the case of the *one-dimensional* situation and $s \geq \frac{1}{2}$, it is possible to treat arbitrary potentials which are bounded by scaling-critical Hardy type potentials (with a smallness condition for $s = \frac{1}{2}$). This is a consequence of the explicit estimates on the spectral gap of the extension operator (c.f. Section 3.8).
- We allow for *arbitrarily large scaling-critical potentials*. Furthermore, our subcritical potentials need not be differentiable. In the frequency function framework a regularity restriction was needed in order to deduce Pohozaev identities.
- Our approach allows for generalizations to *variable coefficient problems*. In this sense we can treat “variable coefficient” fractional Laplacian operators, c.f. Section 3.10.

If $s \geq \frac{1}{4}$, our main results are derived as consequences of the following Carleman estimate:

Proposition 13 (Symmetric Carleman Estimate). *Let $s \in [\frac{1}{4}, 1)$ and let*

$$\phi(y) = -\ln(|y|) + \frac{1}{10} \left(\ln(|y|) \arctan(\ln(|y|)) - \frac{1}{2} \ln(1 + \ln(|y|)^2) \right).$$

Consider $w \in H^1(y_{n+1}^{1-2s} dy, \mathbb{R}_+^{n+1})$ with

$$\begin{aligned} \nabla \cdot y_{n+1}^{1-2s} \nabla w &= f \text{ in } \mathbb{R}_+^{n+1}, \\ \lim_{y_{n+1} \rightarrow 0} y_{n+1}^{1-2s} \partial_{n+1} w &= h \text{ on } \mathbb{R}^n. \end{aligned}$$

Then for $\tau \geq \tau_0 > 0$ we have

$$\begin{aligned}
& \left\| e^{\tau\phi} (1 + \ln(|y|)^2)^{-\frac{1}{2}} y_{n+1}^{\frac{1-2s}{2}} \nabla w \right\|_{L^2(\mathbb{R}_+^{n+1})} \\
& + \tau \left\| e^{\tau\phi} (1 + \ln(|y|)^2)^{-\frac{1}{2}} y_{n+1}^{\frac{1-2s}{2}} |y|^{-1} w \right\|_{L^2(\mathbb{R}_+^{n+1})} \\
& + \tau^s \left\| e^{\tau\phi} (1 + \ln(|y|)^2)^{-\frac{1}{2}} |y|^{-s} w \right\|_{L^2(\mathbb{R}^n)} \\
& \lesssim \tau^{-\frac{1}{2}} \left\| e^{\tau\phi} |y| y_{n+1}^{\frac{2s-1}{2}} f \right\|_{L^2(\mathbb{R}_+^{n+1})} + \tau^{\frac{1-2s}{2}} \left\| e^{\tau\phi} |y|^s h \right\|_{L^2(\mathbb{R}^n)}.
\end{aligned} \tag{3.4.2}$$

We remark that in the case of the half-Laplacian our results can be sharpened by using the framework established by Koch and Tataru [KT01a] dealing with equations of the following form:

$$\partial_i g^{ij} \partial_j u = V u + W_1 \nabla u + \nabla W_2 u, \tag{3.4.3}$$

where $V \in c_0(L^{\frac{n}{2}})$, $W_1, W_2 \in l_w^1(L^n)$ (the function spaces are built by a dyadic summation over annuli) and where g^{ij} are Lipschitz perturbations of the Laplacian. Our problem can be phrased in a similar strong unique continuation framework for (degenerate) elliptic operators by considering the evenly reflected Caffarelli extension. In this case we obtain an equation of the form (3.4.3) where $g^{ij} = |y_{n+1}|^{1-2s} id$ is now degenerate (unless $s = \frac{1}{2}$), $V = 0$ and $W_1 = (0, \dots, 0, H(y_{n+1}))W(y')$, $W_2 = H(y_{n+1})W(y')$ are Heaviside functions at the boundary. Hence, in the case of the half-Laplacian, the strong unique continuation problem can directly be treated with the methods of Koch and Tataru if $V \in l_w^1(L^{n+1})$. Via an improved extension, c.f. Section 3.9, we show that this still remains true for $V \in L^{n+\epsilon}$. For the general fractional Laplacian it appears to be more difficult to reduce the integrability requirements on the potentials via similar means, since the symmetric operator in the Carleman estimates does not yield sufficiently strong positivity anymore.

Last but not least, we would like to stress that our strategy does not only apply to the fractional Laplacian but also works for a much larger class of operators. For any boundary value problem such that the underlying operator

- allows for a sufficiently strong Carleman inequality at the boundary,
- allows for sufficiently strong boundary estimates,

our strategy can be used to derive the strong unique continuation property.

3.5 The Weak Unique Continuation Property

As a first step towards the strong unique continuation result for the fractional operator, we recall the weak unique continuation property for the fractional Laplacian.

Proposition 14 (Weak Unique Continuation). *Let $s \in (0, 1)$ and let $u : \mathbb{R}^n \rightarrow \mathbb{R}$, $u \in H^s(\mathbb{R}^n)$, solve*

$$\begin{aligned} (-\Delta)^s u &= Vu \text{ on } \mathbb{R}^n, \\ u &= 0 \text{ on } \mathbb{R}^n \cap B_1(0). \end{aligned}$$

Then $u \equiv 0$.

Although this property follows from the work of Fall and Felli, c.f. [FF13], by considering the case $V = 0$, we provide an argument for it and strengthen the result to a local statement on the Caffarelli-Silvestre extension. More precisely, we show:

Proposition 15. *Let $s \in (0, 1)$ and let $\tilde{u} \in H_{loc}^1(y_{n+1}^{1-2s} dy, B_1^+(0)) \cap L^\infty(B_1^+(0))$ solve*

$$\begin{aligned} \nabla \cdot y_{n+1}^{1-2s} \nabla \tilde{u} &= 0 \text{ in } B_1^+(0), \\ \lim_{y_{n+1} \rightarrow 0} y_{n+1}^{1-2s} \partial_{n+1} \tilde{u} &= 0 \text{ on } B_1^+(0) \cap \{y_{n+1} = 0\}. \end{aligned} \quad (3.5.1)$$

Further, assume that $\tilde{u}(y', 0) = 0$ on $B_1^+(0) \cap \{y_{n+1} = 0\}$. Then $\tilde{u} \equiv 0$ in $B_1^+(0)$.

In order to see this, we make use of the equation and regularity estimates for the Caffarelli-Silvestre extension. These ingredients can be combined in a boot strap argument.

Proof. We first point out the following two facts:

1. The regularity theory for $H_{loc}^1(y_{n+1}^{1-2s} dy, B_1^+(0)) \cap L^\infty(B_1^+(0))$ weak solutions of

$$\begin{aligned} \nabla \cdot y_{n+1}^{1-2s} \nabla \tilde{u} &= 0 \text{ in } B_1^+(0), \\ \lim_{y_{n+1} \searrow 0} y_{n+1}^{1-2s} \partial_{n+1} \tilde{u} &= f \text{ on } B_1^+(0) \cap \{y_{n+1} = 0\}, \end{aligned} \quad (3.5.2)$$

implies that if $f \in C^{0,\alpha}(B_1(0) \cap \{y_{n+1} = 0\})$, then $y_{n+1}^{1-2s} \partial_{n+1} \tilde{u} \in C^{0,\beta}(\overline{B_{\frac{3}{4}}^+(0)})$ and

$$\|y_{n+1}^{1-2s} \partial_{n+1} \tilde{u}\|_{C^{0,\beta}(\overline{B_{\frac{3}{4}}^+(0)})} \leq C_1,$$

with $C_1 = C_1(s, n, \|f\|_{L^\infty(B_1 \cap \{y_{n+1}=0\})}, \|f\|_{C^{0,\alpha}(B_1(0) \cap \{y_{n+1}=0\})})$. This follows, for example, from the article by Cabré and Sire [CS13].

2. For $a \in (-\infty, 1)$ the mean value theorem and the fundamental theorem of calculus imply that for $u \in C^1((0, 1)) \cap C^0([0, 1])$ the assumptions

$$u(0) = 0 \text{ and } \lim_{y \searrow 0} y^a u'(y) = 0,$$

result in $\lim_{y \searrow 0} y^{a-1} u(y) = 0$.

Step 1: Beginning of the Iteration. We make use of the equation: For this we note that the boundary conditions in (3.5.1) allow to carry out an even reflection and interpret the solution as a $H_{loc}^1(|y_{n+1}|^{1-2s}dy, B_1(0)) \cap L^\infty(B_1(0))$ solution of

$$\nabla \cdot |y_{n+1}|^{1-2s} \nabla \tilde{u} = 0 \text{ in } B_1(0). \quad (3.5.3)$$

For some $\alpha \in (0, 1)$ it is $C^{0,\alpha}$ -regular (in any direction) and C^∞ -smooth in the tangential directions [CS07] (quantitative estimates follow, for example, by carrying out a tangential Fourier transform and treating the remaining equation as an ODE in the normal variable). Thus, it is possible to differentiate (3.5.3) with respect to the tangential directions up to an arbitrary order. Using the continuity of, for instance, $|y_{n+1}|^{1-2s} \partial_{n+1} \Delta' \tilde{u}$ (in $B_{\frac{3}{4}}(0)$) and recalling the even reflection, we obtain

$$\lim_{y_{n+1} \searrow 0} y_{n+1}^{1-2s} \partial_{n+1} \Delta' \tilde{u} = 0. \quad (3.5.4)$$

By the second preliminary remark from above, this leads to

$$\lim_{y_{n+1} \searrow 0} y_{n+1}^{-2s} \Delta' \tilde{u} = 0 \text{ and } y_{n+1}^{-2s} \Delta' u \in C^{0,\gamma}(B_{\frac{3}{4}}(0)). \quad (3.5.5)$$

Hence, we can employ equation (3.5.1) to deduce

$$\lim_{y_{n+1} \searrow 0} \partial_{n+1} y_{n+1}^{1-2s} \partial_{n+1} \tilde{u} = - \lim_{y_{n+1} \searrow 0} y_{n+1}^{1-2s} \Delta' \tilde{u} = 0.$$

For later use, we highlight that this implies

$$\lim_{y_{n+1} \searrow 0} y_{n+1}^{-2s} \partial_{n+1} \tilde{u} = \lim_{y_{n+1} \searrow 0} y_{n+1}^{-2s-1} \tilde{u} = 0.$$

Step 2: Iteration. With the previous considerations, it is possible to differentiate (3.5.1) in the y_{n+1} -direction and consider a weak solution of

$$\begin{aligned} \Delta(y_{n+1}^{1-2s} \partial_{n+1} \tilde{u}) &= -(1-2s)y_{n+1}^{-2s} \Delta' \tilde{u} \text{ in } B_{\frac{3}{4}}^+(0), \\ \lim_{y_{n+1} \searrow 0} \partial_{n+1}(y_{n+1}^{1-2s} \partial_{n+1} \tilde{u}) &= 0 \text{ on } B_{\frac{3}{4}}^+(0) \cap \{y_{n+1} = 0\}. \end{aligned} \quad (3.5.6)$$

Using the observations (3.5.4) and (3.5.5), this leads to

$$\begin{aligned} \lim_{y_{n+1} \searrow 0} \partial_{n+1}^2 y_{n+1}^{1-2s} \partial_{n+1} \tilde{u} &= -(1-2s) \lim_{y_{n+1} \searrow 0} y_{n+1}^{-2s} \partial_{n+1} \tilde{u} \\ &\quad - \lim_{y_{n+1} \searrow 0} y_{n+1}^{1-2s} \partial_{n+1} \Delta' \tilde{u} = 0. \end{aligned}$$

Therefore,

$$\lim_{y_{n+1} \searrow 0} \partial_{n+1}^2 y_{n+1}^{1-2s} \partial_{n+1} \tilde{u} = \lim_{y_{n+1} \searrow 0} y_{n+1}^{-2s-2} \tilde{u} = 0.$$

As before, we need to complement this by limiting behaviour of tangential deriva-

tives in order to estimate the contributions in the new right hand sides of a differentiated version of (3.5.6). We obtain this by reflecting the function $w(y) := y_{n+1}^{1-2s} \partial_{n+1} \tilde{u}$ evenly onto the whole unit ball. In analogy to the previous considerations from step 1, it solves an equation of the type (3.5.6) in the whole unit ball. We differentiate in the tangential directions. For instance, if we consider second tangential derivatives, this implies the continuity of $\partial_{n+1} \Delta' w$, which then results in $\lim_{y_{n+1} \searrow 0} \partial_{n+1} \Delta' w = 0$ (for this we also use higher order analogues of (3.5.5) which follow from taking higher order tangential derivatives in step 1). By virtue of the second remark from above and the definition of w , this implies

$$\lim_{y_{n+1} \searrow 0} \partial_{n+1} y_{n+1}^{1-2s} \partial_{n+1} \Delta' \tilde{u} = \lim_{y_{n+1} \searrow 0} y_{n+1}^{-2s} \partial_{n+1} \Delta' \tilde{u} = \lim_{y_{n+1} \searrow 0} y_{n+1}^{-2s-1} \Delta' \tilde{u} = 0.$$

These terms, however, exactly form the right hand side contributions which result from differentiating (3.5.6) in the normal direction once more. Thus, a bootstrap argument is possible.

Step 3: Conclusion. Using the bootstrap procedure, we obtain

$$\lim_{y_{n+1} \searrow 0} y_{n+1}^{-m} \tilde{u} = 0$$

for all $m \in \mathbb{N}$, i.e. \tilde{u} vanishes of infinite order in the normal direction at $y = 0$. Combined with the vanishing in the tangential direction and the Carleman inequality from Proposition 13, this yields $u \equiv 0$ in $B_1^+(0)$. \square

Remark 11. If $s = \frac{1}{2}$, the statement of the proposition follows from the weak unique continuation property of the $(n+1)$ -dimensional Laplacian. This can be seen by extending the Caffarelli-Silvestre extension, \tilde{u} , trivially in the negative y_{n+1} -direction.

3.6 Symmetric Carleman Estimates

3.6.1 Conformal Coordinates

In order to prove the desired Carleman inequality, we carry out a change of coordinates similar as in [KT01a].

Starting from polar coordinates, the degenerate elliptic operator $\nabla \cdot y_{n+1}^{1-2s} \nabla$ reads

$$\theta_n^{1-2s} \frac{1}{r^n} \partial_r (r^{n+1-2s} \partial_r) + r^{-1-2s} \nabla_{S^n} \cdot \theta_n^{1-2s} \nabla_{S^n},$$

where $\theta_n = \frac{y_{n+1}}{|y|} = \sin(\varphi)$. We transform into conformal coordinates, i.e. $r = e^t$, which yields $\partial_r = e^{-t} \partial_t$. This leads to

$$e^{-(1+2s)t} \left[\theta_n^{1-2s} \partial_t^2 + (n-2s) \theta_n^{1-2s} \partial_t + \nabla_{S^n} \cdot \theta_n^{1-2s} \nabla_{S^n} \right].$$

Conjugating with $e^{-\frac{n-2s}{2}t}$ (which corresponds to setting $w = e^{-\frac{n-2s}{2}t}u$) and multiplying the operator with $e^{(1+2s)t}$, results in

$$\theta_n^{1-2s} \left(\partial_t^2 - \frac{(n-2s)^2}{4} \right) + \nabla_{S^n} \cdot \theta_n^{1-2s} \nabla_{S^n}. \quad (3.6.1)$$

In the case of $s = \frac{1}{2}$ this corresponds to the situation in [KT01a].

In the sequel we will be using several changes of coordinates. In order to avoid confusion, we clarify the conventions we will be adhering to:

Remark 12 (Notation). In the proof of Proposition 13 (and in the remaining text)

- we use w to denote the original function in Cartesian variables,
- after a change to conformal coordinates u is obtained from w via $u(e^t, \theta) = e^{\frac{n-2s}{2}t} w(e^t, \theta)$,
- v is deduced from u by multiplying with the normal variable: $v = \theta_n^{\frac{1-2s}{2}} u$.

Proof of Proposition 13. Step 1: Change of coordinates. We carry out a change of coordinates, as this simplifies the handling of the duality formulation of the equation: We set $v = \theta_n^{\frac{1-2s}{2}} u$ and multiply (3.6.1) with $\theta_n^{\frac{2s-1}{2}}$ from the left. In this formulation the conjugated version of equation (3.6.1) turns into

$$\begin{aligned} e^{\varphi(t)} \left(\partial_t^2 - \frac{(n-2s)^2}{4} + \theta_n^{\frac{2s-1}{2}} \nabla_{S^n} \cdot \theta_n^{1-2s} \nabla_{S^n} \theta_n^{\frac{2s-1}{2}} \right) e^{-\varphi(t)} v &= \theta_n^{\frac{2s-1}{2}} f, \\ \lim_{\theta_n \rightarrow 0} \theta_n^{1-2s} \nu \cdot \nabla_{S^n} \theta_n^{\frac{2s-1}{2}} v &= h, \end{aligned} \quad (3.6.2)$$

where $\varphi = \tau\phi$. In the new coordinates the desired Carleman inequality (3.4.2) then reads

$$\begin{aligned} &\tau^{-\frac{1}{2}} \left\| (\varphi''(t))^{\frac{1}{2}} \theta_n^{\frac{1-2s}{2}} \nabla_{S^n} \theta_n^{\frac{2s-1}{2}} v \right\|_{L^2(\mathbb{R} \times S_+^n)} + \tau^{-\frac{1}{2}} \left\| (\varphi''(t))^{\frac{1}{2}} \partial_t v \right\|_{L^2(\mathbb{R} \times S_+^n)} \\ &+ \tau^{\frac{1}{2}} \left\| (\varphi''(t))^{\frac{1}{2}} v \right\|_{L^2(\mathbb{R} \times S_+^n)} + \tau^{\frac{2s-1}{2}} \left\| (\varphi''(t))^{\frac{1}{2}} \lim_{\theta_n \rightarrow 0} \theta_n^{\frac{2s-1}{2}} v \right\|_{L^2(\mathbb{R} \times \partial S_+^n)} \\ &\lesssim \tau^{-\frac{1}{2}} \left\| \theta_n^{\frac{2s-1}{2}} f \right\|_{L^2(\mathbb{R} \times S_+^n)} + \tau^{\frac{1-2s}{2}} \|h\|_{L^2(\mathbb{R} \times \partial S_+^n)} \quad \text{for } \tau \geq \tau_0 > 0. \end{aligned}$$

We test equation (3.6.2) with eigenfunctions of the spherical operator

$$\theta_n^{\frac{2s-1}{2}} \nabla_{S^n} \cdot \theta_n^{1-2s} \nabla_{S^n} \theta_n^{\frac{2s-1}{2}}$$

with vanishing generalized Neumann data. Then equation (3.6.2) turns into

$$e^{\varphi(t)} \left(\partial_t^2 - \lambda^2 - \frac{(n-2s)^2}{4} \right) e^{-\varphi(t)} E_\lambda v = E_\lambda \theta_n^{\frac{2s-1}{2}} f + \tilde{E}_\lambda h,$$

where we denote the projection of a function v onto the eigenvector v_λ by $E_\lambda v$ and its weighted boundary projection by $\tilde{E}_\lambda v$. With a slight abuse of notation we will

also use the symbol $\tilde{E}_\lambda v$ for the scalar $\int_{\partial S_+^n} v \lim_{\theta_n \rightarrow 0} \theta_n^{\frac{1-2s}{2}} v_\lambda d\mathcal{H}^{n-1}$.

The existence of a countable, diverging sequence of eigenvalues for the spatial part of the operator (3.6.2) follows from the compactness of its inverse operator in an appropriate function space which is defined in the next step of the proof.

Step 2: An Adapted Space. We define the analogues of the spaces \dot{H}^1 with the aid of our equation. Instead of the space \dot{H}^1 , we use the modified space \dot{H}_θ^1 :

$$\dot{H}_\theta^1 := \left\{ v \mid \left\| \theta_n^{\frac{1-2s}{2}} \nabla_{S^n} \theta_n^{\frac{2s-1}{2}} v \right\|_{L^2(\mathbb{R} \times S_+^n)} + \|\partial_t v\|_{L^2(\mathbb{R} \times S_+^n)} < \infty \right\},$$

and its semi-norm

$$\begin{aligned} \|v\|_{\dot{H}_\theta^1} &= \|v\|_{\dot{H}_{\theta,1}^1} + \|v\|_{\dot{H}_{\theta,2}^1} \quad \text{with} \\ \|v\|_{\dot{H}_{\theta,1}^1} &= \left\| \theta_n^{\frac{1-2s}{2}} \nabla_{S^n} \theta_n^{\frac{2s-1}{2}} v \right\|_{L^2(\mathbb{R} \times S_+^n)}, \quad \|v\|_{\dot{H}_{\theta,2}^1} = \|\partial_t v\|_{L^2(\mathbb{R} \times S_+^n)}. \end{aligned}$$

We remark that intersected with $L_{loc}^2(\mathbb{R} \times S_+^n)$ (and augmented by the right boundary values), this space constitutes the natural setting for the weak formulation of (3.6.2). Due to the compactness of the embedding $H^1(\theta_n^{1-2s}, S_+^n) \hookrightarrow L^2(\theta_n^{1-2s}, S_+^n)$, the solution operator associated with the vanishing Neumann version of the spherical operator contained in (3.6.2) is compact if we additionally impose a mean value condition on the spaces (more precisely, the mean value property should be phrased as $\int_{S_+^n} \theta_n^{\frac{2s-1}{2}} v d\theta = 0$). As a result, its inverse has the claimed sequence of diverging eigenvalues.

Step 3: A trace estimate. A key tool in obtaining the desired Carleman estimates consists of using the right trace estimates. We use the following interpolation inequality:

Lemma 6. *Let $s \in (0, 1)$ and let $u : S_+^n \rightarrow \mathbb{R}$ be measurable. Then,*

$$\|u\|_{L^2(S^{n-1})} \lesssim \tau^{1-s} \left\| \theta_n^{\frac{1-2s}{2}} u \right\|_{L^2(S_+^n)} + \tau^{-s} \left\| \theta_n^{\frac{1-2s}{2}} \nabla_{S^n} u \right\|_{L^2(S_+^n)} \quad (3.6.3)$$

for $\tau > 1$.

Proof. By Herbst's inequality (or the Hardy-trace inequality) we have

$$\left\| |y'|^{-s} w_1 \right\|_{L^2(\mathbb{R}^n)} \lesssim \left\| y_{n+1}^{\frac{1-2s}{2}} \nabla w_1 \right\|_{L^2(\mathbb{R}_+^{n+1})},$$

with $y = (y', y_{n+1})$, $y' \in \mathbb{R}^n$ and $s \in (0, 1)$. Applied to functions supported in $B_1^+(0)$ this leads to

$$\|w_1\|_{L^2(B_1(0))} \lesssim \left\| y_{n+1}^{\frac{1-2s}{2}} \nabla w_1 \right\|_{L^2(B_1^+(0))} + \left\| y_{n+1}^{\frac{1-2s}{2}} w_1 \right\|_{L^2(B_1^+(0))}.$$

Rescaling, i.e. setting $w_1(x) = w(\mu x)$, yields

$$\|w\|_{L^2(B_\mu(0))} \lesssim \mu^{s-1} \left\| y_{n+1}^{\frac{1-2s}{2}} w \right\|_{L^2(B_\mu^+(0))} + \mu^s \left\| y_{n+1}^{\frac{1-2s}{2}} \nabla w \right\|_{L^2(B_\mu^+(0))}.$$

From this, it is possible to obtain the multiplicative form of the inequality:

$$\|w\|_{L^2(B_\mu(0))} \lesssim \left\| y_{n+1}^{\frac{1-2s}{2}} w \right\|_{L^2(B_\mu^+(0))}^s \left\| y_{n+1}^{\frac{1-2s}{2}} \nabla w \right\|_{L^2(B_\mu^+(0))}^{1-s},$$

which – by scaling – can be applied to arbitrary functions in $C_0^\infty(\mathbb{R}_+^{n+1})$. As a consequence, we obtain the estimate

$$\|w\|_{L^2(B_\mu(0))} \lesssim \tau^{1-s} \left\| y_{n+1}^{\frac{1-2s}{2}} w \right\|_{L^2(B_\mu^+(0))} + \tau^{-s} \left\| y_{n+1}^{\frac{1-2s}{2}} \nabla w \right\|_{L^2(B_\mu^+(0))},$$

for all $\mu \geq 0$. It remains to localize this estimate to the sphere. This can be achieved by extending an arbitrary function $u : S_+^n \rightarrow \mathbb{R}$ zero-homogeneously into a neighbourhood of S_+^n . Using a cut-off function η , we apply the previous estimate to $w = \eta \tilde{u}$, where \tilde{u} corresponds to the (zero-homogeneous) extension of u . This results in

$$\begin{aligned} \|u\|_{L^2(S^{n-1})} &\lesssim \|w\|_{L^2(\mathbb{R}^n)} \\ &\lesssim \tau^{-s} \left\| y_{n+1}^{\frac{1-2s}{2}} \nabla \tilde{u} \right\|_{L^2(B_2^+ \setminus B_{\frac{1}{2}}^+)} + (\tau^{-s} + \tau^{1-s}) \left\| y_{n+1}^{\frac{1-2s}{2}} \tilde{u} \right\|_{L^2(B_2^+ \setminus B_{\frac{1}{2}}^+)} \\ &\lesssim \tau^{-s} \left\| y_{n+1}^{\frac{1-2s}{2}} \nabla_{S_+^n} u \right\|_{L^2(S_+^n)} + \tau^{1-s} \left\| y_{n+1}^{\frac{1-2s}{2}} u \right\|_{L^2(S_+^n)}, \end{aligned}$$

for $\tau > 1$. □

Step 4: Conclusion. We conclude the argument with a commutator estimate: After the projection onto the eigenvectors, the operator becomes purely one-dimensional

$$\begin{aligned} LE_\lambda v &:= \left(\partial_t^2 + (\varphi'(t))^2 - 2\varphi'(t)\partial_t - \varphi''(t) - \lambda^2 - \frac{(n-2s)^2}{4} \right) E_\lambda v \\ &= -\tilde{E}_\lambda h + E_\lambda \theta_n^{\frac{2s-1}{2}} f. \end{aligned}$$

It decomposes into a symmetric and an antisymmetric part. Setting $\mu^2 := \lambda^2 + \frac{(n-2s)^2}{4}$ leads to

$$\begin{aligned} S &= \partial_t^2 + (\varphi')^2 - \mu^2, \\ A &= -2\varphi'\partial_t - \varphi''. \end{aligned}$$

As its commutator reads

$$\int_{\mathbb{R}} ([S, A]E_\lambda v, E_\lambda v) dt = \int_{\mathbb{R}} \varphi''(\varphi')^2 (E_\lambda v)^2 + \varphi''(E_\lambda v')^2 - \varphi''''(E_\lambda v)^2 dt,$$

we obtain the estimate

$$\begin{aligned} \|LE_\lambda v\|_{L^2(\mathbb{R})}^2 &\geq \|SE_\lambda v\|_{L^2(\mathbb{R})}^2 + \|AE_\lambda v\|_{L^2(\mathbb{R})}^2 + \int_{\mathbb{R}} ([S, A]E_\lambda v, E_\lambda v) dt \\ &\geq \|(\partial_t^2 + \varphi'^2 - \mu^2)E_\lambda v\|_{L^2(\mathbb{R})}^2 + \|(2\varphi'\partial_t + \varphi'')E_\lambda v\|_{L^2(\mathbb{R})}^2 \\ &\quad + \int_{\mathbb{R}} \varphi''(\varphi')^2(E_\lambda v)^2 + \varphi''(E_\lambda v')^2 - \varphi''''(E_\lambda v)^2 dt. \end{aligned}$$

By assumption φ is a convex weight of the form $\varphi(t) = -\tau t + \tau\psi$ and $\psi''(t) = \frac{1}{10(1+t^2)}$. Hence, we observe that the first two commutator contributions are positive and it is possible to absorb the potentially negative $\varphi''''(E_\lambda v)^2$ contribution of the commutator in the other positive contributions. Therefore, we obtain

$$\left\|(\varphi'')^{\frac{1}{2}}\varphi'E_\lambda v\right\|_{L^2(\mathbb{R})} + \left\|(\varphi'')^{\frac{1}{2}}E_\lambda v'\right\|_{L^2(\mathbb{R})} \lesssim \|LE_\lambda v\|_{L^2(\mathbb{R})}. \quad (3.6.4)$$

Moreover, we note that in the regimes $\lambda \geq 4\tau$ and $\lambda \leq \frac{\tau}{2}$ the symmetric part of the operator is elliptic (where the symbol of the operator is interpreted as a symbol in the t - and τ -variables), as by virtue of the definition of the weight function $|\varphi'| \in [\frac{3}{4}\tau, 2\tau]$. Hence, by scaling we also obtain

$$\lambda^2 \|E_\lambda v\|_{L^2(\mathbb{R})} + \lambda \|E_\lambda v'\|_{L^2(\mathbb{R})} \lesssim \|LE_\lambda v\|_{L^2(\mathbb{R})} \quad (3.6.5)$$

in these two elliptic regimes. By definition of the space \dot{H}_θ^1 , it holds

$$\|E_\lambda v\|_{\dot{H}_\theta^1(S_+^n)} = \lambda \|E_\lambda v\|_{L^2(S_+^n)}.$$

Integrating the estimates (3.6.4) and (3.6.5) over S_+^n , shows

$$\left\|(\varphi'')^{\frac{1}{2}}(\varphi')E_\lambda v\right\|_{\dot{H}_\theta^1(S_+^n)L_t^2(\mathbb{R})} \lesssim \|LE_\lambda v\|_{L^2(S_+^n \times \mathbb{R})}.$$

Thus, these estimates yield the bulk contributions of the left hand side of the Carleman inequality.

We proceed by estimating the contributions on the right hand side of the Carleman inequality:

$$\|LE_\lambda v\|_{L^2(S_+^n \times \mathbb{R})} \leq \|E_\lambda f\|_{L^2(S^n \times \mathbb{R})} + \left\|\tilde{E}_\lambda h\right\|_{L^2(\partial S^n \times \mathbb{R})}.$$

In this context, it suffices to discuss the second term. It can be estimated via the trace inequality:

$$\left\|\tilde{E}_\lambda h\right\|_{L^2(\partial S^n \times \mathbb{R})} \leq \lambda^{1-s} \|E_\lambda h\|_{L^2(S^n \times \mathbb{R})}.$$

In the low and critical frequency regimes, i.e. if $\lambda \leq 4\tau$, this can be estimated by $\tau^{1-s} \|E_\lambda h\|_{L^2(S^n \times \mathbb{R})}$. In the high frequency regime, we can also replace the λ factor

by τ , as then the estimates become elliptic, e.g. the L^2 bulk estimate (with $f = 0$) then reads

$$\|E_\lambda v\|_{L^2(S_+^n \times \mathbb{R})} \lesssim \lambda^{-1-s} \|E_\lambda h\|_{L^2(S_+^n \times \mathbb{R})} \lesssim \tau^{-1-s} \|E_\lambda h\|_{L^2(S_+^n \times \mathbb{R})}.$$

The other contributions can be treated analogously. Combined with the previous considerations this implies the estimate

$$\begin{aligned} & \tau^{-\frac{1}{2}} \left\| (\varphi''(t))^{\frac{1}{2}} \theta_n^{\frac{1-2s}{2}} \nabla_{S^n} \theta_n^{\frac{2s-1}{2}} v \right\|_{L^2(\mathbb{R} \times S_+^n)} + \tau^{-\frac{1}{2}} \left\| (\varphi''(t))^{\frac{1}{2}} \partial_t v \right\|_{L^2(\mathbb{R} \times S_+^n)} \\ & + \tau^{\frac{1}{2}} \left\| (\varphi''(t))^{\frac{1}{2}} v \right\|_{L^2(\mathbb{R} \times S_+^n)} \\ & \lesssim \tau^{-\frac{1}{2}} \left\| \theta_n^{\frac{2s-1}{2}} f \right\|_{L^2(\mathbb{R} \times S_+^n)} + \tau^{\frac{1-2s}{2}} \|h\|_{L^2(\mathbb{R} \times \partial S_+^n)}. \end{aligned}$$

Now, the estimate on the boundary contributions follows from the interpolation inequality (3.6.3) applied to $u = \theta_n^{\frac{2s-1}{2}} v$, Fubini's theorem and the condition $|\varphi'| \in [\frac{3}{4}\tau, 2\tau]$:

$$\begin{aligned} \tau^s \left\| (\varphi''(t))^{\frac{1}{2}} \lim_{\theta_n \rightarrow 0} \theta_n^{\frac{2s-1}{2}} v \right\|_{L^2(\mathbb{R} \times \partial S_+^n)} & \lesssim \left\| (\varphi''(t))^{\frac{1}{2}} (\varphi') v \right\|_{L^2(\mathbb{R}^2)} + \left\| (\varphi''(t))^{\frac{1}{2}} v' \right\|_{L^2(\mathbb{R}^2)} \\ & \lesssim \|LE_\lambda v\|_{L^2(\mathbb{R})}. \end{aligned}$$

This yields the full result. \square

Before deducing further results from this, we pause for a few remarks:

Remark 13 (Spectral Gap). The equations (3.6.1) and (3.6.2) contain the structure of the operator in its cleanest form:

$$\begin{aligned} \tilde{\Delta} & := \partial_t^2 - \frac{(n-2s)^2}{4} + \theta_n^{-\frac{1-2s}{2}} \nabla_{S^n} \cdot \theta_n^{1-2s} \nabla_{S^n} \theta_n^{-\frac{1-2s}{2}} \\ & =: \partial_t^2 - \frac{(n-2s)^2}{4} - \tilde{\Delta}_\theta. \end{aligned} \tag{3.6.6}$$

The corresponding boundary values turn into

$$\lim_{\theta_n \rightarrow 0} \theta_n^{1-2s} \nu \cdot \nabla_{S^n} \theta_n^{-\frac{1-2s}{2}} v = e^{2st} \lim_{\theta_n \rightarrow 0} \theta_n^{-\frac{1-2s}{2}} V v.$$

At first sight, one could hope that the eigenvalue expansion of the spherical operator leads to a situation comparable to that of Koch and Tataru [KT01a]. However, this is not clear. As the θ_n -factors break the full rotation symmetry, the spectral gap of the spherical Laplacian need not be preserved.

We note that *in the case* of a spectral gap of constant strength, the Carleman

inequality, (3.4.2), can be further improved by an estimate of the form

$$\begin{aligned} & \text{dist}(\varphi'(t), \text{spec}(\tilde{\Delta}_\theta)) \left\| \theta_n^{\frac{1-2s}{2}} u \right\|_{L^2(\mathbb{R} \times S_+^n)} \\ & \lesssim \tau^{-\frac{1}{2}} \left\| \theta_n^{\frac{2s-1}{2}} f \right\|_{L^2(\mathbb{R} \times S_+^n)} + \tau^{\frac{1-2s}{2}} \|h\|_{L^2(\mathbb{R} \times \partial S_+^n)}. \end{aligned}$$

A similar remark holds for the gradient inequality. This type of estimates can, for example, be seen by constructing a parametrix for the operator

$$e^{-\varphi(t)} \left(\partial_t^2 - \frac{(n-2s)^2}{4} - \tilde{\Delta}_\theta \right) e^{\varphi(t)}$$

on each eigenspace. Following Koch and Tataru [KT01a], using $\varphi'(t) \leq 0$, $\varphi''(t) > 0$ and setting

$$\mu = \sqrt{\frac{(n-2s)^2}{4} + \lambda^2},$$

the kernel of this parametrix reads

$$K_\mu(t, s) = e^{\varphi(t) - \varphi(s)} \begin{cases} -\frac{1}{2} \mu^{-1} e^{-\mu|t-s|} & \text{if } t > T(\mu), \\ \mu^{-1} \sinh(\mu(s-t)) & \text{if } T(\mu) > t > s, \\ 0 & \text{if } T(\mu), s > t, \end{cases}$$

on the eigenspace associated with the eigenvalue μ . Here $T(\mu)$ is a solution of

$$\varphi'(t) = -\mu,$$

if μ is in the range of φ' and else is defined as

$$T(\mu) = \begin{cases} -\infty & \text{if } -\mu < \varphi', \\ +\infty & \text{if } -\mu > \varphi'. \end{cases}$$

Thus, using convexity, the kernel can be estimated by

$$|K_\mu(t, s)| \leq \tau^{-1} e^{-\text{dist}(\varphi'(t), \mu)|t-s|}$$

in the critical regime in which $\varphi' \in [\frac{\tau}{2}, 4\tau]$. Combined with Young's inequality and the estimates in the low and high frequency elliptic regimes, this implies the claimed L^2 bound. We will use this for the one-dimensional fractional Laplacian, c.f. Section 3.8.

Remark 14. From the antisymmetric part of the operator we can obtain further L^2 bounds in combination with Poincaré's inequality. Using the same notation as in Remark 12 and in the proof of Proposition 13, we assume that w is supported in $\{\delta \leq |y| \leq R\}$ or in other words, v is supported in $\{\ln(\delta) \leq t \leq \ln(R)\} \times S_+^n$. Then, for $0 < c_0 < c < C_0 < \infty$ and $R \geq C_0 \delta$, the antisymmetric operator can be

estimated from below

$$\begin{aligned}
\|Av\|_{L^2((\ln(\delta), \ln(R)) \times S_+^n)}^2 &\geq \|Av\|_{L^2((\ln(\delta), \ln(c\delta)) \times S_+^n)}^2 \\
&= \tau^2 \|(2\partial_t \phi \partial_t + \partial_t^2 \phi)v\|_{L^2((\ln(\delta), \ln(c\delta)) \times S_+^n)}^2 \\
&\gtrsim \tau^2 \|(\partial_t \phi) \partial_t v\|_{L^2((\ln(\delta), \ln(c\delta)) \times S_+^n)}^2 \\
&\quad - \tau^2 \|(\partial_t^2 \phi)v\|_{L^2((\ln(\delta), \ln(c\delta)) \times S_+^n)}^2.
\end{aligned}$$

While considering the second quantity in this inequality as a controlled error contribution, we further estimate the first one. Using

$$\partial_t \phi \partial_t v = \partial_t (\partial_t \phi v) - \partial_t^2 \phi v$$

as well as $\partial_t v|_{(e^t, \theta)} = e^{-t} \partial_t g|_{(t, \theta)}$ with $g(t, \theta) = v(e^t, \theta)$ in combination with Poincaré's inequality leads to:

$$\begin{aligned}
\|Av\|_{L^2((\ln(\delta), \ln(R)) \times S_+^n)}^2 &\gtrsim \tau^2 \delta^{-2} \|\partial_t \phi v\|_{L^2((\ln(\delta), \ln(c\delta)) \times S_+^n)}^2 \\
&\quad - 2\tau^2 \|(\partial_t^2 \phi)v\|_{L^2((\ln(\delta), \ln(c\delta)) \times S_+^n)}^2.
\end{aligned}$$

Recalling the proof of the Carleman estimate (3.4.2), we observe that the right hand side of the inequality, in particular, bounds the antisymmetric part of the operator. In v -variables and using $\varphi = \tau\phi$, this amounts to the estimate

$$\begin{aligned}
&\tau^{-\frac{1}{2}} \left\| (\varphi''(t))^{\frac{1}{2}} \theta_n^{\frac{1-2s}{2}} \nabla_{S^n} \theta_n^{\frac{2s-1}{2}} v \right\|_{L^2(\mathbb{R} \times S_+^n)} + \tau^{-\frac{1}{2}} \left\| (\varphi''(t))^{\frac{1}{2}} \partial_t v \right\|_{L^2(\mathbb{R} \times S_+^n)} \\
&+ \tau^{\frac{1}{2}} \left\| (\varphi''(t))^{\frac{1}{2}} v \right\|_{L^2(\mathbb{R} \times S_+^n)} + \tau^{-\frac{1}{2}} \|(2\varphi'(t) + \varphi''(t))v\|_{L^2(\mathbb{R} \times S_+^n)} \\
&+ \tau^{\frac{2s-1}{2}} \left\| (\varphi''(t))^{\frac{1}{2}} \lim_{\theta_n \rightarrow 0} \theta_n^{\frac{2s-1}{2}} v \right\|_{L^2(\mathbb{R} \times \partial S_+^n)} \\
&\lesssim \tau^{-\frac{1}{2}} \left\| \theta_n^{\frac{2s-1}{2}} f \right\|_{L^2(\mathbb{R} \times S_+^n)} + \tau^{\frac{1-2s}{2}} \|h\|_{L^2(\mathbb{R} \times \partial S_+^n)} \quad \text{for } \tau \geq \tau_0 > 0.
\end{aligned}$$

Hence, as the error term can be absorbed in the Carleman inequality, the estimate from above corresponds to

$$\tau^2 \delta^{-2} \left\| e^{\tau\phi} y_{n+1}^{\frac{1-2s}{2}} w \right\|_{L^2(B_{c\delta} \setminus B_\delta)}^2 \lesssim \left\| e^{\tau\phi} y_{n+1}^{\frac{2s-1}{2}} |y| \nabla \cdot y_{n+1}^{1-2s} \nabla w \right\|_{L^2(B_R \setminus B_\delta)}^2$$

in Cartesian coordinates (if $h = 0$).

3.6.2 Consequences of the Carleman Estimate (3.4.2)

From the previous estimates we obtain a unique continuation result in the case of infinite order vanishing in both the tangential and normal directions.

Corollary 1 (SUCP I). *Let $s \in (0, 1)$ and let $w : \mathbb{R}^n \rightarrow \mathbb{R}$, $w \in H^s$, be a solution*

of

$$(-\Delta)^s w = Vw,$$

with $V = V_1 + V_2$,

$$V_1(y) = |y|^{-2s} h \left(\frac{y}{|y|} \right), \quad h \in L^\infty, \quad |V_2(y)| \leq c|y|^{-2s+\epsilon}.$$

For $s < \frac{1}{2}$, we additionally require that one of the following assumptions is satisfied:

- the potential V_2 satisfies $V_2 \in C^1(\mathbb{R}^n \setminus \{0\})$ and $|y \cdot \nabla V_2| \lesssim c|y|^{-2s+\epsilon}$,
- $s \in [\frac{1}{4}, \frac{1}{2})$ and $V_1 \equiv 0$.

Let \tilde{w} denote the Caffarelli extension of w . If \tilde{w} vanishes of infinite order at 0 in both the tangential and normal directions, then

$$w \equiv 0.$$

Remark 15. Before presenting the proof, we deduce an estimate for (critically) weighted boundary terms, involving e.g. $V(y) \sim |y|^{-2s}$. Due to the infinite order of vanishing of w along the boundary, for any $\epsilon > 0$ and any $m \in \mathbb{N}$, there exists a radius $\bar{r} = \bar{r}(m, \epsilon) > 0$ such that for all $0 < r \leq \bar{r}$

$$\int_{B_{2r} \setminus B_r} |V|w^2 dy \lesssim r^{-2s} \int_{B_{2r} \setminus B_r} w^2 dy \leq \epsilon r^m.$$

As a result,

$$\begin{aligned} \int_{B_{2r}} |V|w^2 dy &= \sum_{j \in \mathbb{N}} \int_{B_{2^{-j}r} \setminus B_{2^{-j-1}r}} |V|w^2 dy \\ &\lesssim \epsilon r^m \sum_{j \in \mathbb{N}} 2^{-jm} \\ &\lesssim \epsilon r^m. \end{aligned}$$

Hence, the infinite rate of vanishing of u on the boundary also implies that (singularly) weighted boundary integrals have an infinite rate of vanishing.

We present the proof for subcritically scaling potentials in the case $s \geq \frac{1}{4}$ first. Then we indicate how to modify the previous arguments for $0 < s < \frac{1}{4}$ and in the case of scale-invariant potentials.

Proof in the Case of Subcritical Potentials and $s \geq \frac{1}{4}$. Step 1: Interpolation. For

$w \in C_0^\infty(\overline{Q_\epsilon^+})$ and $0 \leq \epsilon \leq \frac{1}{2}$ the following interpolation inequality holds true:

$$\begin{aligned} \frac{1}{\epsilon^2} \int_{Q_\epsilon^+} y_{n+1}^{1-2s} |\nabla w|^2 dy &\lesssim \frac{C(\mu)}{\epsilon^4} \int_{Q_\epsilon^+} y_{n+1}^{1-2s} |w|^2 dy + \mu^2 \int_{Q_\epsilon^+} y_{n+1}^{2s-1} |\nabla \cdot y_{n+1}^{1-2s} \nabla w|^2 dy \\ &\quad - \frac{1}{\epsilon^2} \int_{Q_\epsilon^+ \cap \{y_{n+1}=0\}} w y_{n+1}^{1-2s} \partial_{n+1} w dy', \end{aligned}$$

where $Q_\epsilon^+ = [-\epsilon, \epsilon]^n \times [0, \epsilon]$. This estimate will be employed in deriving the infinite order of vanishing of the gradient from the infinite order of vanishing of $\frac{1}{\epsilon^4} \int_{B_\epsilon} y_{n+1}^{1-2s} w^2 dy$ for (almost) solutions.

The inequality is a result of integration by parts and the support condition on w . In fact, we have

$$\int_{Q_1^+} y_{n+1}^{1-2s} |\nabla' w|^2 dy = - \int_0^1 y_{n+1}^{1-2s} \int_{[-1,1]^n} w \Delta' w(\cdot, y_{n+1}) dy' dy_{n+1}.$$

Moreover,

$$\begin{aligned} \int_{Q_1^+} y_{n+1}^{1-2s} |\partial_{n+1} w|^2 dy &= - \int_{[-1,1]^n} \int_0^1 w (\partial_{n+1} y_{n+1}^{1-2s} \partial_{n+1} w) dy_{n+1} dy' \\ &\quad - \int_{[-1,1]^n \times \{0\}} w y_{n+1}^{1-2s} \partial_{n+1} w dy'. \end{aligned}$$

Combining these two estimates yields

$$\begin{aligned} \int_{Q_1^+} y_{n+1}^{1-2s} |\nabla w|^2 dy &\leq \int_{Q_1^+} |w \nabla \cdot y_{n+1}^{1-2s} \nabla w| dy + \int_{[-1,1]^n \times \{0\}} w y_{n+1}^{1-2s} \partial_{n+1} w dy \\ &\leq \mu^2 \int_{Q_1^+} y_{n+1}^{2s-1} |\nabla \cdot y_{n+1}^{1-2s} \nabla w|^2 dy + C(\mu) \int_{Q_1^+} y_{n+1}^{1-2s} |w|^2 dy \\ &\quad - \int_{[-1,1]^n \times \{0\}} w y_{n+1}^{1-2s} \partial_{n+1} w dy. \end{aligned}$$

The claimed inequality now follows from scaling.

Step 2: Cut-off Errors. Denoting the Caffarelli extension of w by \tilde{w} , we consider $\bar{w} = \tilde{w} \eta_{\delta,r}$ where $\eta_{\delta,r}$ is a radial cut-off function which equals one on an annulus with radii approximately determined by δ and r where $0 < \delta \ll r < 1$. Thus, \bar{w}

satisfies

$$\begin{aligned} \nabla \cdot y_{n+1}^{1-2s} \nabla \bar{w} &= y_{n+1}^{1-2s} \eta''_{\delta,r} \tilde{w} + y_{n+1}^{1-2s} \eta'_{\delta,r} \frac{y}{|y|} \cdot \nabla \tilde{w} \\ &\quad + (n+1-2s) y_{n+1}^{1-2s} \frac{1}{|y|} \eta'_{\delta,r} \tilde{w} \text{ in } \mathbb{R}^{n+1}, \quad (3.6.7) \\ - \lim_{y_{n+1} \rightarrow 0} y_{n+1}^{1-2s} \partial_{n+1} \bar{w} &= V \bar{w} \text{ on } \mathbb{R}^n. \end{aligned}$$

Due to the cut-off, it is an admissible function in the Carleman inequality of Proposition 13. Inserting it into the Carleman inequality, we notice that we may pass to the limit $\delta \rightarrow 0$: This follows from step 1 (in which μ is chosen sufficiently small) and the infinite order of vanishing of \bar{w} . Hence, the only remaining cut-off is at the scale $r > 0$.

Step 3: Conclusion for Potentials with Subcritical Scaling. We consider the different contributions of the Carleman inequality:

$$\begin{aligned} &\left\| e^{\tau\phi} (1 + \ln(|y|)^2)^{-\frac{1}{2}} y_{n+1}^{\frac{1-2s}{2}} \nabla w \right\|_{L^2(\mathbb{R}_+^{n+1})} \\ &\quad + \tau \left\| e^{\tau\phi} (1 + \ln(|y|)^2)^{-\frac{1}{2}} y_{n+1}^{\frac{1-2s}{2}} |y|^{-1} w \right\|_{L^2(\mathbb{R}_+^{n+1})} \\ &\quad + \tau^s \left\| e^{\tau\phi} (1 + \ln(|y|)^2)^{-\frac{1}{2}} |y|^{-s} w \right\|_{L^2(\mathbb{R}^n)} \\ &\lesssim \tau^{-\frac{1}{2}} \left\| e^{\tau\phi} |y| y_{n+1}^{\frac{2s-1}{2}} f \right\|_{L^2(\mathbb{R}_+^{n+1})} + \tau^{\frac{1-2s}{2}} \left\| e^{\tau\phi} |y|^s h \right\|_{L^2(\mathbb{R}^n)}. \end{aligned}$$

As all the right hand side terms of (3.6.7) involve derivatives of $\eta_{0,r}$ (which are, in particular, only active at scales $r > 0$), they can be treated as controlled perturbations. Thus, it remains to investigate the boundary contributions. We recall $|V(y)| \leq |y|^{-2s+\epsilon}$. This leads to a boundary contribution of

$$\tau^s \left\| (1 + \ln(|y|)^2)^{-\frac{1}{2}} |y|^{-s} w \right\|_{L^2}$$

on the left hand side of the Carleman inequality, and a contribution of the form

$$\tau^{\frac{1-2s}{2}} \left\| |y|^s h \right\|_{L^2} \lesssim \tau^{\frac{1-2s}{2}} \left\| |y|^{-s+\epsilon} w \right\|_{L^2}, \quad (3.6.8)$$

on the right hand side of the Carleman estimate. We note that in the case $s \geq \frac{1}{4}$ the τ contributions on the right hand side of the Carleman estimate are smaller or equal to the τ contributions on the left hand side. Thus, a strategy in which the dangerous terms of the right hand side are absorbed in the left hand side of the Carleman inequality is possible. By virtue of the choice of the cut-off $\eta_{0,r}$, it suffices to consider $|y| < r$. Due to the subcriticality of V and as the loss on the left hand side of the Carleman inequality is only logarithmic, the term on the right hand side of (3.6.8) can be absorbed in the left hand side of the Carleman inequality. In the limit $\tau \rightarrow \infty$ this yields the desired result for (rough) subcritical potentials. \square

In the sequel, we comment on the proof of Corollary 1 in the case $s \in (0, \frac{1}{4})$ and in the setting involving scale-invariant potentials. For this, we argue via slightly different methods in obtaining the crucial Carleman estimates: In contrast to the previous arguments we do not carry out a decomposition into the spherical eigenvalues but work with the full operator.

Proof for $s \in (0, \frac{1}{2})$ and for Scaling-Critical Potentials. Step 1: Conjugation and bulk contributions. We carry out the Carleman argument without projecting onto eigenvalues of the spherical operator. We start with the operator in conformal coordinates

$$\partial_t^2 - \frac{(n-2s)^2}{4} + \theta_n^{-\frac{1-2s}{2}} \nabla_{S^n} \cdot \theta_n^{1-2s} \nabla_{S^n} \theta_n^{-\frac{1-2s}{2}}.$$

Conjugation with an only t -dependent weight ϕ , leads to the following symmetric and antisymmetric parts of the operator:

$$S = \partial_t^2 + \tau^2 (\partial_t \phi)^2 - \frac{(n-2s)^2}{4} + \theta_n^{-\frac{1-2s}{2}} \nabla_{S^n} \cdot \theta_n^{1-2s} \nabla_{S^n} \theta_n^{-\frac{1-2s}{2}},$$

$$A = -2\tau (\partial_t \phi) \partial_t - \tau \partial_t^2 \phi.$$

If ϕ is sufficiently pseudoconvex this yields positive commutator terms. Furthermore, weighted gradient estimates can be obtained:

$$\begin{aligned} & ((\partial_t^2 \phi) \partial_t v, \partial_t v) + ((\partial_t^2 \phi) \theta_n^{1-2s} \nabla_{S^n} \theta_n^{-\frac{1-2s}{2}} v, \nabla_{S^n} \theta_n^{-\frac{1-2s}{2}} v) \\ &= - (Sv, (\partial_t^2 \phi) v) + \int_{\partial S_+^n \times \mathbb{R}} (\partial_t^2 \phi) \theta_n^{1-2s} (\nu \cdot \nabla_{S^n} \theta_n^{-\frac{1-2s}{2}} v) \theta_n^{-\frac{1-2s}{2}} v d\theta dt + ((\partial_t^4 \phi) v, v) \\ &\leq \frac{1}{2\tau^2} \|Sv\|_{L^2}^2 + \frac{1}{2} \tau^2 \|(\partial_t^2 \phi) v\|_{L^2}^2 + \tau^2 \left\| (\partial_t^2 \phi)^{\frac{1}{2}} \partial_t v \right\|_{L^2}^2 - \frac{(n-2)^2}{4} \left\| (\partial_t^2 \phi)^{\frac{1}{2}} v \right\|_{L^2}^2 \\ &\quad + \int_{\partial S_+^n \times \mathbb{R}} (\partial_t^2 \phi) \theta_n^{1-2s} (\nu \cdot \nabla_{S^n} \theta_n^{-\frac{1-2s}{2}} v) \theta_n^{-\frac{1-2s}{2}} v d\theta dt + ((\partial_t^4 \phi) v, v)_{L^2}, \end{aligned}$$

where $\nu = (0, \dots, 0, -1)$ denotes the outer unit normal. For sufficiently pseudoconvex ϕ the right hand side can be controlled by the commutator contributions of the Carleman estimate. In fact, this can even be strengthened by noticing that the right hand side remains controlled if it is multiplied by a factor of $c\tau$, with c sufficiently small; for example $c \sim \frac{1}{2}$ would work. The boundary integral can be evaluated to yield

$$\int_{\partial S_+^n \times \mathbb{R}} (\partial_t^2 \phi) (\theta_n^{1-2s} \nu \cdot \nabla_{S^n} \theta_n^{-\frac{1-2s}{2}} v) \theta_n^{-\frac{1-2s}{2}} v d\theta dt = \int_{\partial S_+^n \times \mathbb{R}} \theta_n^{-(1-2s)} (\partial_t^2 \phi) e^{2st} V v^2 d\theta dt.$$

The remaining boundary integral which originates from the commutator calculation

is given by

$$\begin{aligned}
& 4\tau \int_{\partial S_+^n \times \mathbb{R}} \theta_n^{1-2s} (\nu \cdot \nabla_{S^n} \theta_n^{-\frac{1-2s}{2}} v) (\partial_t \phi) \theta_n^{-\frac{1-2s}{2}} \partial_t v d\theta dt \\
& + 2\tau \int_{\partial S_+^n \times \mathbb{R}} \theta_n^{1-2s} (\nu \cdot \nabla_{S^n} \theta_n^{-\frac{1-2s}{2}} v) (\partial_t^2 \phi) \theta_n^{-\frac{1-2s}{2}} v d\theta dt \\
& = 4\tau \int_{\partial S_+^n \times \mathbb{R}} (\partial_t \phi) \theta_n^{-(1-2s)} e^{2st} V v \partial_t v d\theta dt + 2\tau \int_{\partial S_+^n \times \mathbb{R}} (\partial_t^2 \phi) \theta_n^{-(1-2s)} e^{2st} V v^2 d\theta dt.
\end{aligned}$$

Rewritten in terms of $u = \theta_n^{-\frac{1-2s}{2}} v$ the Carleman estimate reads

$$\begin{aligned}
& c\tau \left\| (\partial_t^2 \phi)^{\frac{1}{2}} \theta_n^{\frac{1-2s}{2}} \partial_t u \right\|_{L^2}^2 + c\tau \left\| (\partial_t^2 \phi)^{\frac{1}{2}} \theta_n^{\frac{1-2s}{2}} \nabla_{S^n} u \right\|_{L^2}^2 + c\tau^3 \left\| \theta_n^{\frac{1-2s}{2}} (\partial_t^2 \phi)^{\frac{1}{2}} (\partial_t \phi) u \right\|_{L^2}^2 \\
& + \left\| S(\theta_n^{\frac{1-2s}{2}} u) \right\|_{L^2}^2 + \tau^{-1} \left\| (\partial_t^2 + \theta_n^{-\frac{1-2s}{2}} \nabla_{S^n} \cdot \theta_n^{1-2s} \nabla_{S^n} \theta_n^{-\frac{1-2s}{2}}) \theta_n^{\frac{1-2s}{2}} u \right\|_{L^2}^2 \\
& + 4\tau \int_{\partial S_+^n \times \mathbb{R}} (\partial_t \phi) e^{2st} V u \partial_t u d\theta dt + 2\tau \int_{\partial S_+^n \times \mathbb{R}} (\partial_t^2 \phi) e^{2st} V u \partial_t u d\theta dt \\
& + c\tau \int_{\partial S_+^n \times \mathbb{R}} (\partial_t^2 \phi) e^{2st} V u \partial_t u d\theta dt \\
& \leq \|L_\phi u\|_{L^2}^2,
\end{aligned}$$

where

$$\begin{aligned}
L_\phi &= \theta_n^{\frac{1-2s}{2}} (\partial_t^2 + \tau^2 (\partial_t \phi)^2) - \frac{(n-2s)^2}{4} - 2\tau (\partial_t \phi) \partial_t - \tau \partial_t^2 \phi \\
& + \theta_n^{-\frac{1-2s}{2}} \nabla_{S^n} \cdot \theta_n^{1-2s} \nabla_{S^n}.
\end{aligned}$$

Inserting the changes we made, i.e. $w = e^{\frac{n-2s}{2}t} u$, and recalling the changes in the volume element, yields a Carleman inequality which, up to the boundary contributions, is comparable to (3.4.2).

Step 2: Boundary Contributions under Differentiability Assumptions. In order to obtain a unique continuation statement as in Corollary 1, it remains to deal with the boundary contributions. We first present the argument under the differentiability assumption

$$V_2 \in C^1(\mathbb{R}^n \setminus \{0\}), \quad |y \cdot \nabla V_2| \leq c|y|^{-2s+\epsilon},$$

independently of the value of $s \in (0, 1)$. In order to estimate the unsigned boundary contributions, we consider the respective expressions in u -coordinates. Starting with

the scaling-critical Hardy potentials, we have to bound

$$\begin{aligned} & 4\tau \int_{\partial S_+^n \times \mathbb{R}} (\partial_t \phi) e^{2st} V_1 u \partial_t u d\theta dt + 2\tau \int_{\partial S_+^n \times \mathbb{R}} (\partial_t^2 \phi) e^{2st} V_1 u^2 d\theta dt \\ & + c\tau \int_{\partial S_+^n \times \mathbb{R}} (\partial_t^2 \phi) e^{2st} V_1 u^2 d\theta dt, \end{aligned}$$

i.e. we have to control the boundary integrals involving the potential $V_1 = e^{-2st} h(\theta)$. By an integration by parts in t , we obtain that most contributions drop out. Indeed, the only non-vanishing term is given by

$$c\tau \int_{\partial S_+^n \times \mathbb{R}} \partial_t^2 \phi h(\theta) u^2 d\theta dt.$$

This can be controlled via the interpolation inequality (3.6.3):

$$\tau \int_{\partial S_+^n \times \mathbb{R}} (\partial_t^2 \phi) h(\theta) u^2 d\theta dt \lesssim \tau^{1-s} \left\| (\partial_t^2 \phi)^{\frac{1}{2}} \theta_n^{\frac{1-2s}{2}} \nabla_{S^n} u \right\|_{L^2}^2 + \tau^{2-s} \left\| \theta_n^{\frac{1-2s}{2}} (\partial_t^2 \phi)^{\frac{1}{2}} u \right\|_{L^2}^2.$$

All the remaining boundary contributions involve the potential V_2 which has subcritical growth at zero. Due to the form of ϕ , it suffices to deduce control of the term

$$4\tau \int_{\partial S_+^n \times \mathbb{R}} \partial_t \phi e^{2st} V_2 u \partial_t u d\theta dt.$$

Integrating by parts in t , using the subcriticality of V_2 and the properties of ϕ , it suffices to bound

$$C\tau \int_{\partial S_+^n \times \mathbb{R}} e^{\epsilon t} u^2 d\theta dt.$$

As the condition on the support of u implies that $t < 0$, this can once more be achieved via the interpolation inequality (3.6.3).

Step 3: Scaling-Critical Potentials for $s \geq \frac{1}{2}$. Last but not least, we indicate how to prove the desired Carleman estimate in cases involving scaling-critical potentials without the differentiability assumptions from the previous step. While the scaling-critical potential, V_1 , can be treated as the potentials in step 2, the subcritical part of the potential, V_2 , cannot be differentiated. Thus, a direct estimate of this boundary term is needed. This is achieved via interpolation and regularity estimates for the operators. We only present the argument for the most critical boundary contribution which (after localization to a small radius $0 < r \ll 1$) in Cartesian

coordinates reads:

$$\tau \int_{B_r^+ \cap \{y_{n+1}=0\}} |V_2| |w(y \cdot \nabla w)| dy.$$

We estimate

$$\begin{aligned} \tau \int_{B_r^+ \cap \{y_{n+1}=0\}} |V_2| |w(y \cdot \nabla w)| dy &\lesssim \tau^2 \int_{B_r^+ \cap \{y_{n+1}=0\}} |y|^{-2s+\epsilon} w^2 dy \\ &+ \int_{B_r^+ \cap \{y_{n+1}=0\}} |y|^{2-2s+\epsilon} |\nabla w|^2 dy. \end{aligned} \quad (3.6.9)$$

The first term can directly be interpolated between controlled quantities:

$$\tau^2 \int_{B_r^+ \cap \{y_{n+1}=0\}} |y|^{-2s+\epsilon} w^2 dy \lesssim \tau \left\| |y|^{\frac{\epsilon}{2}} y_{n+1}^{\frac{1-2s}{2}} \nabla w \right\|_{L^2(B_r^+)} + \tau^3 \left\| |y|^{\frac{\epsilon}{2}-1} y_{n+1}^{\frac{1-2s}{2}} w \right\|_{L^2(B_r^+)}.$$

Here we have used $s \in [\frac{1}{2}, 1)$. The second quantity in (3.6.9) has to be controlled using elliptic estimates. Due to L^2 estimates for the respective degenerate elliptic Neumann boundary value problem (which one can for example deduce by carrying out a tangential Fourier transform), we have

$$\begin{aligned} &\int_{B_r^+ \cap \{y_{n+1}=0\}} |y|^{2-2s+\epsilon} |\nabla w|^2 dy \\ &\lesssim \tau^{-1} \left\| |y|^{1+\frac{\epsilon}{2}} (y_{n+1}^{\frac{2s-1}{2}} \nabla \cdot y_{n+1}^{1-2s} \nabla + \tau^2 |\nabla \phi|^2 y_{n+1}^{\frac{1-2s}{2}}) w \right\|_{L^2(B_{2r}^+)}^2 \\ &+ \tau^2 \left\| |y|^{-1+\frac{\epsilon}{2}} y_{n+1}^{\frac{1-2s}{2}} w \right\|_{L^2(B_{2r}^+)}^2 + \tau \left\| |y|^{\frac{\epsilon}{2}} y_{n+1}^{\frac{1-2s}{2}} \nabla w \right\|_{L^2(B_{2r}^+)}^2 \\ &+ \tau^{2-4s} \left\| |y|^{s+\frac{\epsilon}{2}} V w \right\|_{L^2(B_{2r}^+ \cap \{y_{n+1}=0\})}^2. \end{aligned}$$

As all the right hand side terms are controlled by the bulk terms of the Carleman inequality, we can also control perturbations of critically scaling potentials without imposing differentiability constraints on the perturbation. \square

3.7 Doubling Estimates and Reduction to the Weak Unique Continuation Property

3.7.1 Doubling Inequalities

In this section we deduce a doubling inequality which plays a decisive role in the compactness argument reducing the strong to the weak unique continuation property. We have

Proposition 16. *Let $s \in (0, 1)$ and let $w : \mathbb{R}^{n+1} \rightarrow \mathbb{R}$, $w \in H_{loc}^1(y_{n+1}^{1-2s} dy, \mathbb{R}^{n+1}) \cap$*

$H_{loc}^2(y_{n+1}^{1-2s} dy, \mathbb{R}^{n+1})$, be a solution of

$$\begin{aligned} \nabla \cdot y_{n+1}^{1-2s} \nabla w &= 0 \text{ in } \mathbb{R}_+^{n+1}, \\ - \lim_{y_{n+1} \rightarrow 0} y_{n+1}^{1-2s} \partial_{n+1} w &= Vw \text{ on } \mathbb{R}^n, \end{aligned}$$

with $V = V_1 + V_2$,

$$V_1(y) = |y|^{-2s} h\left(\frac{y}{|y|}\right), \quad h \in L^\infty, \quad |V_2(y)| \leq c|y|^{-2s+\epsilon}.$$

For $s < \frac{1}{2}$, we additionally require that one of the following assumptions is satisfied:

- the potential V_2 satisfies $V_2 \in C^1(\mathbb{R}^n \setminus \{0\})$ and $|y \cdot \nabla V_2| \lesssim c|y|^{-2s+\epsilon}$,
- $s \in [\frac{1}{4}, \frac{1}{2})$ and $V_1 \equiv 0$.

Then the doubling property holds, i.e. there exists a constant $C > 0$ and a constant R such that for all $0 < r < R$ we have

$$\left\| y_{n+1}^{\frac{1-2s}{2}} w \right\|_{L^2(B_{2r}^+(0))} \leq C \left\| y_{n+1}^{\frac{1-2s}{2}} w \right\|_{L^2(B_r^+(0))}.$$

Before commencing with the proof of the doubling property, a few remarks are in order:

Remark 16. • We note that the doubling property can be shown for any $R > 0$. However, in order to obtain a uniform dependence of C on r , this parameter has to be fixed.

- We point out that the constant $C > 0$ depends on the function w .
- The doubling property is neither restricted to balls centered at the origin nor to balls centered at the boundary of \mathbb{R}_+^{n+1} . Under the conditions of Proposition 16 the conclusion can be formulated as the existence of a constant $C > 0$ and a constant R such that for all $0 < r < R$ and for all $y_0 \in B_R(z)$, $z \in \mathbb{R}_+^{n+1}$, we have

$$\left\| y_{n+1}^{\frac{1-2s}{2}} w \right\|_{L^2(B_{2r}(y_0) \cap \mathbb{R}_+^{n+1})} \leq C \left\| y_{n+1}^{\frac{1-2s}{2}} w \right\|_{L^2(B_r(y_0) \cap \mathbb{R}_+^{n+1})}.$$

In this case $C = C(R, z, w)$. We comment on the proof of this more general statement after the proof of Proposition 16, c.f. Remark 17.

Proof. Without loss of generality, we restrict our attention to sufficiently small radii and to balls centered at the origin. Via a covering argument, it is possible to recover the statement for larger balls, c.f. Remark 17. In order to bound the gradient contributions which will arise in the application of the Carleman inequality (3.4.2), we recall the following elliptic gradient/ Caccioppoli estimate: Let ψ be a cut-off function supported in an annulus given by $0 < \frac{r_0}{2} \leq |y| \leq 2r_1 < \infty$, which

we will also denote by $(\frac{r_0}{2}, 2r_1)$ in the sequel. Then,

$$\begin{aligned} \left\| y_{n+1}^{\frac{1-2s}{2}} \nabla(w\psi) \right\|_{L^2(\frac{r_0}{2}, 2r_1)}^2 &\lesssim r_0^{-2} \left\| y_{n+1}^{\frac{1-2s}{2}} w \right\|_{L^2(r_0/2, 2r_1)}^2 \\ &+ \int_{(\frac{r_0}{2}, 2r_1) \cap \{y_{n+1}=0\}} \psi w \lim_{y_{n+1} \rightarrow 0} y_{n+1}^{1-2s} \partial_{n+1}(\psi w) dy, \end{aligned} \quad (3.7.1)$$

with $0 < r_0 < r_1 < \infty$. If the boundary conditions are of the generalized Neumann type as in our assumptions, it becomes possible to absorb these into the left-hand side bulk gradient term, if they are sufficiently small, i.e. if V is either subcritical or if it is a small scaling-critical potential. In the case of large scaling-critical potentials it is still possible to absorb these contributions, if the vanishing rate in the tangential direction is higher than in the normal direction. By virtue of Corollary 1 it is always possible to reduce to this situation.

Keeping this in mind, we prepare for the application of the Carleman inequality from Proposition 13: Let η be a radial cut-off function, which is equal to one on the annulus $|y| \in (\delta, \tilde{R}/2)$ and vanishes outside of the annulus $|y| \in (\delta/2, \tilde{R})$. Inserting ηw into the Carleman estimate (in combination with Remark 14), using the elliptic estimate as well as the explicit form of the boundary contribution, we obtain

$$\begin{aligned} &\delta^{-2} \tau \left\| e^{\tau\phi} y_{n+1}^{\frac{1-2s}{2}} w \right\|_{L^2(\delta, 3\delta)}^2 \\ &+ \tau^2 \tilde{R}^{-2} \left\| e^{\tau\phi} (1 + \ln(|y|)^2)^{-\frac{1}{2}} y_{n+1}^{\frac{1-2s}{2}} w \right\|_{L^2(\tilde{R}/8, \tilde{R}/4)}^2 \\ &\lesssim \delta^{-2} \left\| e^{\tau\phi} y_{n+1}^{\frac{1-2s}{2}} w \right\|_{L^2(\delta/2, \frac{3\delta}{2})}^2 + \tilde{R}^{-2} \left\| e^{\tau\phi} y_{n+1}^{\frac{1-2s}{2}} w \right\|_{L^2(\tilde{R}/2, 2\tilde{R})}^2. \end{aligned}$$

Here the boundary contributions were absorbed into the bulk contributions in the way indicated above. Setting $\tilde{R} \sim 1$, we estimate further

$$\begin{aligned} &e^{\tau\phi(3\delta)} \left\| y_{n+1}^{\frac{1-2s}{2}} w \right\|_{L^2(B_{3\delta})}^2 + e^{\tau\phi(\tilde{R}/4)} \delta^2 \tau^2 \left\| y_{n+1}^{\frac{1-2s}{2}} w \right\|_{L^2(\tilde{R}/8, \tilde{R}/4)}^2 \\ &\lesssim \delta^2 e^{\tau\phi(\tilde{R}/2)} \left\| y_{n+1}^{\frac{1-2s}{2}} w \right\|_{L^2(B_{2\tilde{R}})}^2 + e^{\tau\phi(\frac{\delta}{2})} \left\| y_{n+1}^{\frac{1-2s}{2}} w \right\|_{L^2(B_{3\delta/2})}^2. \end{aligned}$$

Now, we choose $\tau > 0$ such that $\delta^2 e^{\tau\phi(\tilde{R}/2)} \left\| y_{n+1}^{\frac{1-2s}{2}} w \right\|_{L^2(B_{2\tilde{R}})}^2$ on the right hand side can be absorbed in the term $e^{\tau\phi(\tilde{R}/4)} \tau^2 \delta^2 \left\| y_{n+1}^{\frac{1-2s}{2}} w \right\|_{L^2(\tilde{R}/8, \tilde{R}/4)}^2$ on the left hand side. A possible choice of τ , for example, is

$$\tau \sim \frac{1}{\phi(\tilde{R}/2) - \phi(\tilde{R}/4)} \ln \left(\frac{\left\| y_{n+1}^{\frac{1-2s}{2}} w \right\|_{L^2(\tilde{R}/8, \tilde{R}/4)}}{\left\| y_{n+1}^{\frac{1-2s}{2}} w \right\|_{L^2(B_{2\tilde{R}})}} \right).$$

This implies the doubling inequality for $r = \delta$ with a constant which, by virtue of

the structure of ϕ , does not depend on δ . Since $0 < \delta \ll \tilde{R}$ was arbitrary, this implies the doubling property. \square

Remark 17. The more general claim of Remark 16 follows from two ingredients: a three balls inequality and an overlapping chains argument. The three balls inequality compares the value of w on a ball of size r with balls of size $\frac{r}{2}$ and $2r$:

$$\left\| y_{n+1}^{\frac{1-2s}{2}} w \right\|_{L^2(B_r(y_0) \cap \mathbb{R}_+^{n+1})} \leq C \left\| y_{n+1}^{\frac{1-2s}{2}} w \right\|_{L^2(B_{\frac{r}{2}}(y_0) \cap \mathbb{R}_+^{n+1})}^\alpha \left\| y_{n+1}^{\frac{1-2s}{2}} w \right\|_{L^2(B_{2r}(y_0) \cap \mathbb{R}_+^{n+1})}^{1-\alpha},$$

for sufficiently small radii $r > 0$. This inequality allows to compare the values of w along a chain of overlapping balls. Thus, it is possible to deduce an estimate of the form

$$\left\| y_{n+1}^{\frac{1-2s}{2}} w \right\|_{L^2(B_r(y_0))} \geq C_r \left\| y_{n+1}^{\frac{1-2s}{2}} w \right\|_{L^2(B_{2R}(z))}.$$

Hence, the norms of w on smaller balls can be related to the norms on the whole ball $B_{2R}(z)$. This then allows to deduce the stronger doubling inequality of Remark 16 as well as the reduction to sufficiently small balls in the proof of Proposition 16. For further details we refer to the articles on quantitative unique continuation by Bakri [Bak11].

3.7.2 Reduction to the Weak Unique Continuation Problem

In this section we explain how the previous estimates can be combined in order to reduce the strong unique continuation problem to its weak analogue. The key argument relies on a blow-up procedure.

Proposition 17 (SUCP II). *Let $s \in (0, 1)$ and let $w : \mathbb{R}^{n+1} \rightarrow \mathbb{R}$, $w \in H_{loc}^1(y_{n+1}^{1-2s} dy, \mathbb{R}_+^{n+1})$, be a solution of*

$$\begin{aligned} \nabla \cdot y_{n+1}^{1-2s} \nabla w &= 0 \text{ in } \mathbb{R}_+^{n+1}, \\ - \lim_{y_{n+1} \rightarrow 0} y_{n+1}^{1-2s} \partial_{n+1} w &= Vw \text{ on } \mathbb{R}^n, \end{aligned}$$

with $V = V_1 + V_2$,

$$V_1(y) = |y|^{-2s} h \left(\frac{y}{|y|} \right), \quad h \in L^\infty, \quad |V_2(y)| \leq c|y|^{-2s+\epsilon}.$$

For $s < \frac{1}{2}$, we additionally require that one of the following assumptions is satisfied:

- the potential V_2 satisfies $V_2 \in C^1(\mathbb{R}^n \setminus \{0\})$ and $|y \cdot \nabla V_2| \lesssim c|y|^{-2s+\epsilon}$,
- $s \in [\frac{1}{4}, \frac{1}{2})$ and $V_1 \equiv 0$.

Suppose that $w(\cdot, 0)$ vanishes of infinite order at 0. Then

$$w \equiv 0.$$

Proof. Without loss of generality we may assume that w does not vanish of infinite order in both the normal and tangential directions. We consider a rescaled version of w : Let $0 < \sigma \ll 1$. We define

$$w_\sigma(y) = \frac{w(\sigma y)}{\sigma^{-\frac{n+1}{2}} \sigma^{-\frac{1-2s}{2}} \left\| y_{n+1}^{\frac{1-2s}{2}} w \right\|_{L^2(B_\sigma^+(0))}}.$$

Using the gradient estimate, we obtain

$$\begin{aligned} \left\| y_{n+1}^{\frac{1-2s}{2}} \nabla w \right\|_{L^2(B_\sigma^+)}^2 &\lesssim \frac{1}{\sigma^2} \left\| y_{n+1}^{\frac{1-2s}{2}} w \right\|_{L^2(B_{2\sigma}^+)}^2 + \int_{B_{2\sigma}^+ \cap \{y_{n+1}=0\}} \eta^2 y_{n+1}^{1-2s} w \partial_{n+1} w dy, \\ &\lesssim \frac{1}{\sigma^2} \left\| y_{n+1}^{\frac{1-2s}{2}} w \right\|_{L^2(B_\sigma^+)}^2, \end{aligned}$$

where the last line is a consequence of the doubling inequality as well as the finite order of vanishing of w in the normal direction, c.f. Remark 15: Due to the infinite order of vanishing, the boundary contributions can be absorbed in the other terms for sufficiently small σ . In effect, we have

- $\left\| y_{n+1}^{\frac{1-2s}{2}} w_\sigma \right\|_{L^2(B_1^+)} = 1,$
- $\left\| y_{n+1}^{\frac{1-2s}{2}} \nabla w_\sigma \right\|_{L^2(B_1^+)} \leq C.$

Hence, (along a not relabeled subsequence) we may pass to the limit $\sigma \rightarrow 0$ and obtain $w_\sigma \rightarrow w_0$ strongly in L^2 via Rellich's compactness theorem. As a consequence of the infinite order of vanishing (and the finite order of vanishing in the normal direction), w_σ converges to zero on the boundary. Furthermore, w_0 weakly solves

$$\begin{aligned} \nabla \cdot y_{n+1}^{1-2s} \nabla w_0 &= 0 \text{ in } B_1^+(0), \\ \lim_{y_{n+1} \rightarrow 0} y_{n+1}^{1-2s} \partial_{n+1} w_0 &= 0 \text{ on } B_1^+(0) \cap \{y_{n+1} = 0\}. \end{aligned}$$

Due to the weak unique continuation principle (c.f. Proposition 15), w_0 has to vanish (which contradicts $\left\| y_{n+1}^{\frac{1-2s}{2}} w_0 \right\|_{L^2(B_1^+)} = 1$). \square

3.8 The One-Dimensional Situation

In the case of *one-dimensional* fractional Schrödinger equations it is possible to deduce stronger estimates than in the general case since the eigenvalues of the spherical contribution of the symmetric part of the operator satisfy a spectral gap condition. Moreover, they can be computed explicitly. For a fixed $s \in (0, 1)$ the one-dimensionality of the problem reduces the eigenvalue equation to a one-parameter

family of odes:

$$\left(\frac{\partial^2}{\partial^2 \varphi} + \frac{(1-2s)(1+2s)}{4} \frac{1}{\sin(\varphi)^2} - \frac{(1-2s)^2}{4} \right) v = \lambda v \text{ in } [0, \pi],$$

$$\lim_{\sin(\varphi) \rightarrow 0} \sin(\varphi)^{1-2s} \frac{\partial}{\partial \varphi} \sin(\varphi)^{\frac{2s-1}{2}} v = 0 \text{ on } \{0, \pi\}. \quad (3.8.1)$$

This can be reduced to generalized Legendre equations which allow to determine the admissible values of λ :

Lemma 7. *Let $s \in (0, 1)$. Then the eigenvalues of (3.8.1) are of the form*

$$\lambda_k = -\frac{(1-2s)^2}{4} - \left(k - s + \frac{1}{2} \right)^2, \quad k \in \mathbb{N}_{\geq 0}.$$

Apart from the characterization of the eigenvalues, it is also possible to determine (some of) the associated eigenfunctions explicitly. This boils down to finding appropriate solutions of a generalized Legendre equation:

Lemma 8. *Let $\nu = k - \mu$, $k \in \mathbb{N}_{\geq 0}$, $\mu \in (0, 1)$. Then the generalized Legendre equation*

$$(1-x^2)w''(x) - 2xw'(x) + \left(\nu(\nu+1) - \frac{\mu^2}{1-x^2} \right) w(x) = 0, \quad (3.8.2)$$

has a solution of the form

$$f_\nu^\mu(x) = \frac{P_k(x)}{(1-x^2)^{\mu/2}},$$

where $P_k(x)$ is a polynomial of degree (exactly) k .

Proof of Lemma 8. We consider solutions of the generalized Legendre equation (3.8.2) for our choices of parameters μ and ν . In order to solve the equation, we consider the ansatz

$$w(x) = \frac{P_k(x)}{(1-x^2)^{\mu/2}}.$$

Inserting this into the generalized Legendre equation (3.8.2), results in an equation for the P_k :

$$(1-x^2)P_k''(x) + 2(\mu-1)xP_k'(x) + (k^2 - 2k\mu + k)P_k(x) = 0.$$

For a polynomial ansatz, $P_k(x) = \sum_{j=0}^k \alpha_j x^j$, this turns into a recursion formula for

the coefficients α_j :

$$\begin{aligned} 2\alpha_2 + (k^2 - 2k\mu + k)\alpha_0 &= 0, \\ 6\alpha_3 + (2\mu - 2 + k^2 - 2k\mu + k)\alpha_1 &= 0, \\ (j+1)(j+1)\alpha_{j+2} + (j(j-1) + 2j(\mu-1) + k^2 - 2k\mu + k)\alpha_j &= 0, \text{ if } j \geq 2. \end{aligned} \tag{3.8.3}$$

This yields k equations for the $k+1$ coefficients of the polynomial $P_k(x)$. Due to the restrictions $\mu \in (0, 1)$ and $k \geq 0$, the (coefficient) equations can be solved explicitly if $k \leq 3$. Moreover, we notice that the equation

$$x(x-1) + 2x(\mu-1) + k^2 - 2k\mu + k = 0,$$

has pairs of complex-valued solutions if $k \geq 4$ and $\mu \in (0, 1)$ – but no real ones. Hence, by the last equation in (3.8.3), $a_{j+2} \neq 0$ if $a_j \neq 0$. In effect, it is always possible to find a one-parameter family of solutions of system (3.8.3). For even k this depends on a_0 , while for odd k it depends on a_1 . This proves the claim. \square

Proof of Lemma 7. The general (complex valued) solution of the ODE (3.8.1) is given by

$$\begin{aligned} v(\varphi) &= C_1(\cos^2(\varphi) - 1)^{\frac{1}{4}} P_{\frac{1}{2}(-1 + \sqrt{-1 - 4\lambda + 4s - 4s^2})}^s(\cos(\varphi)) \\ &\quad + C_2(\cos^2(\varphi) - 1)^{\frac{1}{4}} Q_{\frac{1}{2}(-1 + \sqrt{-1 - 4\lambda + 4s - 4s^2})}^s(\cos(\varphi)), \end{aligned} \tag{3.8.4}$$

where $P_\nu^\mu(x)$ and $Q_\nu^\mu(x)$ are Legendre functions of the first and second kind, i.e. solutions of the generalized Legendre equation (3.8.2). In order to be an eigenfunction, the solution has to have vanishing generalized Neumann data. Setting $\nu = k - s = \frac{1}{2}(-1 + \sqrt{-1 - 4\lambda + 4s - 4s^2})$, $k \in \mathbb{N}$, leads to simplifications: According to Lemma 8 there are solutions of the form

$$f_\nu^\mu(\cos(\varphi)) = \frac{P_k(\cos(\varphi))}{\sin(\varphi)^s},$$

where $P_k(x)$ is a polynomial of degree k . Thus, for this choice of ν the general solution (3.8.4) becomes

$$v_k(\varphi) = \sin(\varphi)^{\frac{1-2s}{2}} P_k(\cos(\varphi)).$$

Inserting this into the boundary condition, we infer that these functions do not only satisfy (3.8.2) but also obey the right boundary conditions. Thus, these functions are indeed eigenfunctions of our equation. It remains to show that the corresponding eigenvalues constitute the whole spectrum, i.e. there are no further eigenvalues (which we might have missed by computing only special eigenfunctions). This follows from recurrence relations for the generalized Legendre functions. Setting

$h_\nu^\mu(x) = c_1 P_\nu^\mu(x) + c_2 Q_\nu^\mu(x)$ with $c_1, c_2 \in \mathbb{R}$, we have (c.f. [OLBC10]):

$$\begin{aligned} \sin(\varphi)^{1-2s} \frac{\partial}{\partial \varphi} (\sin(\varphi)^s h_\nu^s(\cos(\varphi))) &= s(\sin(\varphi)^{s-1} \cos(\varphi) h_\nu^s(\cos(\varphi)) \\ &\quad - (\sin(\varphi))^{s-1} [(s - \nu - 1) h_{\nu+1}^s(\cos(\varphi)) \\ &\quad + (\nu + 1) \cos(\varphi) h_\nu^s(\cos(\varphi))]) \\ &= -(\sin(\varphi))^{-s} [\cos(\varphi)(s - \nu - 1) h_\nu^s(\cos(\varphi)) \\ &\quad - (s - \nu - 1) h_{\nu+1}^s(\cos(\varphi))]. \end{aligned}$$

Due to the asymptotics of $Q_\nu^\mu(\cos(\varphi))$ at $\varphi = 0$ (a symbolic Mathematica computation yields $Q_\nu^\mu(\cos(\varphi)) \sim \frac{2^{-s} \pi^2 1 / \sin(\pi s) 1 / \sin(\pi(s+\nu))}{\Gamma(s) \Gamma(-s-\nu) \Gamma(1-s+\nu)}$), it follows that $c_2 = 0$ unless $\nu = k - s$ for $k \in \mathbb{N}_{\geq 0}$, as $P_\nu^\mu(\cos(\varphi))$ satisfies the boundary conditions at $\varphi = 0$ for $\mu \in (0, 1)$ and arbitrary ν . We claim that, in effect, only $\nu = k - s$ is admissible (in particular, none of the $P_\nu^s(\cos(\varphi))$ are admissible for $\nu \neq k - s$). This is a consequence of the connection formulas, c.f. [OLBC10], for Legendre functions:

$$P_\nu^\mu(-x) = -\frac{2}{\pi} \sin((\nu + s)\pi) Q_\nu^\mu(x) + \cos((\nu + s)\pi) P_\nu^\mu(x).$$

Evaluated at $x = \cos(\pi)$, the asymptotics of $Q_\nu^\mu(\cos(\varphi))$ and of $P_\nu^\mu(\cos(\varphi))$ imply that $\nu = k - s$, $k \in \mathbb{N}$, is the only admissible family of parameters. Thus, assuming the validity of the boundary conditions at $\varphi = 0$ and at $\varphi = \pi$ necessarily leads to $\nu = k - s$, $k \in \mathbb{N}$. Combined with the form of ν given in (3.8.4), this determines the possible eigenvalues. \square

Remark 18. The explicit representation of the eigenvalues illustrates that in the one-dimensional situation the spectral gap of the extension problem related to the fractional Laplacian is comparable with the spectral gap for the pure Laplacian (in that case $\lambda = -k^2$, $k \in \mathbb{Z}$).

The characterization of the spectrum of the one-dimensional Caffarelli extension allows to deduce stronger L^2 Carleman estimates similar to the ones in [KT01a]. In particular, it is possible to avoid the logarithmic loss in the Carleman estimate. As a consequence, it is possible to treat the strong unique continuation principle for potentials which are bounded by arbitrary scaling invariant Hardy type potentials:

Proposition 18. *Let $s \in [\frac{1}{2}, 1)$ and let $w \in H^s(\mathbb{R})$ be a solution of*

$$(-\Delta)^s w = Vw \text{ in } \mathbb{R}.$$

Assume that w vanishes of infinite order at the origin and that $|V(y)| \lesssim |y|^{-2s}$ if $s > \frac{1}{2}$ and that $|V(y)| \leq c|y|^{-1}$ for $0 < c \ll 1$ if $s = \frac{1}{2}$. Then $w \equiv 0$.

Sketch of Proof. The proof relies on strengthened Carleman bounds. In the case of a spectral gap, it is possible to give bounds which do not depend on the convexity parameter of the weight in exchange of a loss of half a power of τ , c.f. Remark 13. Roughly speaking, in the u -coordinates, this results in a boundary estimate of the

form

$$\tau^{\frac{2s-1}{2}} \|u\|_{L^2(\mathbb{R} \times \partial S_+^n)} \lesssim \tau^{\frac{1-2s}{2}} \|e^{2st} V u\|_{L^2(\mathbb{R} \times \partial S_+^n)} + \text{bulk contributions.}$$

This explains the slightly modified s -dependence of the estimate. \square

3.9 L^p -Regularity: Understanding the Half-Laplacian in the Framework of Koch & Tataru

As pointed out in the introduction, by an even reflection it is possible to interpret the unique continuation problem for the fractional Laplacian in the framework of Koch and Tataru [KT01a]. The potentials W_1 and W_2 are essentially given by $H(y_{n+1})V(y')$, with $H(y_{n+1})$ denoting a Heaviside function. The result of Koch and Tataru immediately demonstrates that for the half-Laplacian the strong unique continuation property holds with $V \in L^1_w(L^{n+1})$ under additional smallness assumptions as described in [KT01a]. For the half-Laplacian scaling arguments, however, suggest that the critical space is given by potentials $V \in L^n$ (possibly obeying some smallness assumption). Thus, it is natural to pose the question whether this can still be achieved in the framework of Koch and Tataru [KT01a]. As we briefly illustrate below, this is indeed possible for subcritical potentials:

Proposition 19. *Let $w \in H^{\frac{1}{2}}(\mathbb{R}^n)$ be a solution of*

$$(-\Delta)^{\frac{1}{2}} w = V w \text{ in } \mathbb{R}^n.$$

Assume that $V \in L^{n+\epsilon}(\mathbb{R}^n)$ and that w vanishes of infinite order at the origin. Then $w \equiv 0$.

Proof. The proof is based on a refined extension. We consider the following auxiliary problem: Let ϕ denote the harmonic (Neumann) extension of the potential V , i.e.

$$\begin{aligned} \Delta \phi &= 0 \text{ in } \mathbb{R}_+^{n+1}, \\ \partial_{n+1} \phi &= V \text{ on } \{y_{n+1} = 0\}. \end{aligned}$$

Then by regularity of the elliptic Neumann problem

$$\phi \in W^{1+\frac{1}{n+\epsilon}, n+\epsilon}(\mathbb{R}_+^{n+1}).$$

Hence, $\nabla \phi \in W^{\frac{1}{n+\epsilon}, n+\epsilon}$ and by the Sobolev embedding theorem for Besov spaces (c.f. for example [Leo09]), we obtain $\nabla \phi \in L^{n+1+\delta}(\mathbb{R}_+^{n+1})$, with $\delta = \delta(\epsilon)$ being a continuous function in ϵ for sufficiently small $0 \leq \epsilon \ll 1$ and satisfying $\delta \geq 0$, $\delta(0) = 0$. This integrability property is preserved under an even reflection. With a slight abuse of notation the reflected solution then distributionally satisfies

$$\Delta \phi = V \delta_0(y_{n+1}) \text{ in } \mathbb{R}^{n+1}.$$

Reflecting the solution, \tilde{w} , of the Caffarelli extension of (3.4.1) evenly and setting $W = \nabla\phi$, we infer

$$\Delta\tilde{w} = \nabla(W\tilde{w}) - W\nabla\tilde{w} \text{ in } \mathbb{R}^{n+1}.$$

As the previous considerations imply that $W \in L^{n+1+\delta}(\mathbb{R}^{n+1})$, the result of Koch and Tataru can be applied. Their machinery then proves the claim. \square

Remark 19. This reduction to the Koch/Tataru setting suggests that the potential V appearing in the equation for the half-Laplacian should be interpreted as a *gradient* rather than a usual potential for an elliptic problem. In this case one cannot expect to deal with arbitrarily large potentials (in contrast to [Pan92]) as a counterexample by Wolff indicates [Wol93] (exactly scaling-critical potentials represent an exception).

3.10 The Carleman Estimates for Variable Coefficient Operators

In this final section on unique continuation properties of the fractional Laplacian we extend the previous results to operators with variable coefficients and operators on domains which are not half-spaces. The methods we present allow to deal with three situations:

- First, we restrict our attention to the flat half-space, \mathbb{R}_+^{n+1} , but consider a class of more general operators with non-constant metrics:

$$\begin{aligned} (\partial_{n+1} y_{n+1}^{1-2s} \partial_{n+1} + \nabla' \cdot y_{n+1}^{1-2s} a(y') \nabla') w &= 0 \text{ in } \mathbb{R}_+^{n+1}, \\ \lim_{y_{n+1} \rightarrow 0} y_{n+1}^{1-2s} \partial_{n+1} w &= Vw \text{ on } \mathbb{R}^n. \end{aligned}$$

Here $a(y')$ is a tensor which satisfies certain Lipschitz bounds. We note that, in particular, this situation corresponds to generalizations of the Caffarelli-Silvestre extension for variable coefficients. Thus, it is possible to think of the results on these operators as statements on “variable coefficient” fractional Laplacians.

- In the second case, we study the analogous situation on manifolds with sufficiently regular boundaries. As we are only interested in a local statement, we consider the situation in local coordinates in a coordinate patch:

$$\begin{aligned} (\partial_\nu d_{\partial\Omega}(y)^{1-2s} \partial_\nu + \nabla_{tan} \cdot d_{\partial\Omega}(y)^{1-2s} a(y_{tan}) \nabla_{tan}) w &= 0 \text{ in } \Omega, \\ \lim_{d_{\partial\Omega}(y) \rightarrow 0} d_{\partial\Omega}(y)^{1-2s} \partial_\nu w &= Vw \text{ on } \partial\Omega. \end{aligned} \tag{3.10.1}$$

In this context we use ∂_ν to denote the “normal” and ∇_{tan} the “tangential” derivatives in appropriate normal coordinates; $d_{\partial\Omega}(y)$ represents the distance

function with respect to the boundary. This setting can be treated in analogy to the flat situation (here we emphasize that first order contributions which originate from the global formulation via corresponding Laplace Beltrami operators on the manifold represent controllable errors, c.f. step 4 in the proof of Proposition 20). As before, the equation can be interpreted as a generalization of the Caffarelli-Silvestre extension to domains with non-flat boundary.

- Last but not least, we comment on the half-Laplacian and the one-dimensional situation for which stronger results are available due to the presence of the already discussed spectral gap. As a consequence, perturbation techniques as in [KT01a] are available.

Since the second situation can be reduced to the first one, we emphasize the details in the \mathbb{R}_+^{n+1} -case and only point out the modifications in the second situation.

3.10.1 The Half-Space Situation with Variable Coefficients and Differentiability

In this section we address the half-space situation with variable coefficients. In this context, we use the following conventions and notations, c.f. [Jos11]:

- Let (M, g) be a Riemannian manifold of dimension m , assume that $p \in M$, $v \in T_p M$ and let $c_v : [0, \epsilon] \rightarrow M$ be a geodesic with $c_v(0) = p$, $\dot{c}_v(0) = v$. Set $V_p := \{v \in T_p M \mid c_v \text{ is defined on } [0, 1]\}$. Then we define

$$\exp_p : V_p \rightarrow M, \quad v \mapsto c_v(1).$$

If we want to point out the dependence on the metric, we also use the notation $\exp_{g,p}$. We remark that if $T_p M$ is identified with \mathbb{R}^m the exponential map yields a local choice of coordinates.

- Let $(M, g) = (\mathbb{R} \times M, 1 \times g(y'))$. We set $l_g(y) := \sqrt{y_{n+1}^2 + \bar{l}_g(y')^2}$ with $y = (y', y_{n+1})$ and $\bar{l}_g(y')$ being the geodesic distance of y' from the origin with respect to the metric $g(y')$ on \mathbb{R}^n .

With this, we can prove the following Proposition:

Proposition 20 (Variable Coefficient Carleman Estimate). *Suppose that $a : \mathbb{R}^n \rightarrow \mathbb{R}^{n \times n}$ with*

$$\lambda |\xi|^2 \leq \xi \cdot a(y') \xi \leq \Lambda |\xi|^2, \quad 0 < \lambda \leq \Lambda < \infty, \quad a_{ij} = a_{ji}, \quad a \in C^2.$$

Let $s \in [\frac{1}{4}, 1)$ and set

$$\phi(y) = -\ln(l_{a^{-1}}(y)) + \frac{1}{10} \left(\ln(l_{a^{-1}}(y)) \arctan(l_{a^{-1}}(y)) - \frac{1}{2} \ln(1 + \ln(l_{a^{-1}}(y))^2) \right).$$

Assume that $w \in H^1(y_{n+1}^{1-2s} dy, \mathbb{R}_+^{n+1})$ with $\text{supp}(w) \subset \overline{B_r(0)^+}$, $0 < r = r(a) \ll 1$, satisfies

$$\begin{aligned} (\partial_{n+1} y_{n+1}^{1-2s} \partial_{n+1} + \nabla' \cdot y_{n+1}^{1-2s} a(y') \nabla') w &= f \text{ in } \mathbb{R}_+^{n+1}, \\ \lim_{y_{n+1} \rightarrow 0} y_{n+1}^{1-2s} \partial_{n+1} w &= Vw \text{ on } \mathbb{R}^n, \end{aligned}$$

and vanishes of infinite order at 0. Further assume that $V = V_1 + V_2$,

$$\begin{aligned} V_1(y) &= l_{a^{-1}}(y)^{-2s} h \left(\frac{y}{l_{a^{-1}}(y)} \right), \quad h \in L^\infty, \quad |V_2(y)| \leq c l_{a^{-1}}(y)^{-2s+\epsilon}, \\ V_2(y) &\in C^1(\mathbb{R}^n \setminus \{0\}), \quad |\nabla V_2(y)| \leq l_{a^{-1}}(y)^{-2s+\epsilon-1}. \end{aligned}$$

Then for $\tau \geq \tau_0 > 0$ we have

$$\begin{aligned} &\tau^s \left\| e^{\tau\phi} (1 + \ln(l_{a^{-1}}(y))^2)^{-\frac{1}{2}} l_{a^{-1}}(y)^{-s} w \right\|_{L^2(\mathbb{R}^n)} \\ &+ \tau \left\| e^{\tau\phi} (1 + \ln(l_{a^{-1}}(y))^2)^{-\frac{1}{2}} l_{a^{-1}}(y)^{-1} y_{n+1}^{\frac{1-2s}{2}} w \right\|_{L^2(\mathbb{R}_+^{n+1})}^2 \\ &+ \left\| e^{\tau\phi} (1 + \ln(l_{a^{-1}}(y))^2)^{-\frac{1}{2}} y_{n+1}^{\frac{1-2s}{2}} \nabla w \right\|_{L^2(\mathbb{R}_+^{n+1})}^2 \\ &\lesssim \tau^{-\frac{1}{2}} \left\| e^{\tau\phi} l_{a^{-1}}(y) y_{n+1}^{\frac{2s-1}{2}} f \right\|_{L^2(\mathbb{R}_+^{n+1})} + \tau^{\frac{1-2s}{2}} \left\| e^{\tau\phi} l_{a^{-1}}(y)^s Vw \right\|_{L^2(\mathbb{R}^n)}. \end{aligned}$$

Remark 20. • The C^2 regularity condition on the metric is an artifact of our strategy of proof: We make use of the exponential map associated with the metric $a^{-1}(y')$ in order to pass to geodesic polar coordinates. An alternative strategy using arguments from [KT01a] would have been possible. With this method it is possible to reduce to the (optimal) setting of Lipschitz metrics.

- The radius $r > 0$ in the proposition is chosen so small that we may pass to geodesic normal coordinates in it. This is no restriction in general, as it is possible to use appropriate cut-off functions.
- We use the notation $a(y')^{-1}$ to denote the pointwise inverse of $a(y')$, i.e.

$$a(y')^{-1} a(y') = \delta_{ij}.$$

In order to prove the desired Carleman inequality, we carry out a change of coordinates similar to the one described in the article of Koch and Tataru [KT01a]. Working with variable metrics, we have to introduce appropriate normal coordinates first. Thus, we cast our equation into a Riemannian framework where the Riemannian metric g is given by a^{-1} . We note that after the change of coordinates our argument strongly resembles the proof of Corollary 1 in the case of .

Proof of Proposition 20. Step 1: Choice of Coordinates. We cast the equation into a Riemannian framework. In this context we may interpret the tangential part of

the operator as

$$\nabla' \cdot a(y') \nabla' = \Delta'_{a^{-1}} - \frac{1}{2} v_{a^{-1}}(y') \cdot a(y') \nabla' = \Delta'_{a^{-1}} - \frac{1}{2} v_{a^{-1}}(y') \cdot \nabla'_{a^{-1}},$$

where $v_{a^{-1}}(y')$ is a vector with i -th component given by $v_{a^{-1},i}(y') = \text{tr}(a^{-1}(y') \frac{\partial a}{\partial y_i})$. Here $\Delta'_{a^{-1}}$ and $\nabla'_{a^{-1}}$ denote the Laplace-Beltrami and gradient operators with respect to the metric $a(y')^{-1}$. We point out that the thus introduced metric is truly Riemannian as – due to the y' -dependence of a – it depends on the point of evaluation. For the moment, we ignore the first order contribution in the definition of our operator. It can be considered as “small” and can be treated as a controlled error contribution.

With this interpretation of the tangential operator, the full operator can be interpreted as a (degenerate) elliptic operator acting on the Riemannian manifold $(\mathbb{R}_+ \times \mathbb{R}^n, 1 \times a(y')^{-1})$. In this setting, we aim at reducing the situation to geodesic polar coordinates. These can be obtained by first introducing Riemannian normal coordinates in the tangential directions and then passing to (geodesic) polar coordinates in the tangential and normal variables.

We commence by considering the tangential geometry: We may interpret it as the manifold $(\mathbb{R}^n, a_{ij}(y')^{-1})$. Using (the locally well-defined) exponential map, we obtain normal coordinates on an open subset of \mathbb{R}^n (here we make use of the C^2 condition on the metric g). As our Carleman estimates are formulated as local estimates for functions which are supported sufficiently close to zero, we assume that the change of coordinates is a global one and that our new manifold is given by $(\mathbb{R}^n, \bar{g}_{ij})$. This change of coordinates straightens out the geodesics passing through the origin.

Now we consider the full operator in the whole of $(\mathbb{R}_+ \times \mathbb{R}^n, 1 \times \bar{g}_{ij})$ and introduce polar, instead of Cartesian coordinates in \mathbb{R}_+^{n+1} . This leads to a new spherical metric $g_{\theta\theta}$ and to a modified operator:

$$\begin{aligned} & \theta_n^{1-2s} \frac{1}{r^n} \partial_r (r^{n+1-2s} \partial_r) + \theta_n^{1-2s} r^{-1-2s} \frac{1}{2} \text{tr}(g_{\theta\theta} \partial_r g_{\theta\theta}^{-1}) \partial_r \\ & + r^{-1-2s} \frac{1}{\sqrt{\det g_{\theta\theta}}} \partial_{\theta_i} \cdot \theta_n^{1-2s} g_{\theta\theta}^{-1}(r, \theta) \sqrt{\det g_{\theta\theta}} \partial_{\theta_j}. \end{aligned}$$

In the sequel, we will also denote the spherical metric $g_{\theta\theta}(r, \theta)$ by $g(r, \theta)$ and ignore the first order term involving the derivatives of $g_{\theta\theta}$. Due to the smallness of the homogeneous Lipschitz norm of g , it can be treated as a controlled error contribution which can be absorbed in the positive bulk terms.

We carry out the change into conformal coordinates, i.e. $r = e^t$, which yields $\partial_r = e^{-t} \partial_t$. This results in

$$e^{-(1+2s)t} \left[\theta_n^{1-2s} \partial_t^2 + (n-2s) \theta_n^{1-2s} \partial_t + \tilde{\nabla}_{S^n} \cdot \theta_n^{1-2s} \tilde{\nabla}_{S^n} \right],$$

where for brevity of notation we used $\tilde{\nabla}_{S^n}$ to denote the spherical gradient with respect to our (non-standard) spherical metric. Conjugating with $e^{-\frac{n-2s}{2}t}$ (which

corresponds to setting $w = e^{-\frac{n-2s}{2}t}u$ and multiplying the operator with $e^{(1+2s)t}$, results in

$$\theta_n^{1-2s} \left(\partial_t^2 - \frac{(n-2s)^2}{4} \right) + \tilde{\nabla}_{S^n} \cdot \theta_n^{1-2s} \tilde{\nabla}_{S^n}.$$

Due to the product structure of our original manifold, the boundary condition turns into $\lim_{\theta_n \rightarrow 0} \theta_n^{1-2s} \partial_{\varphi_n} u = e^{2st} V u$. In analogy to the flat case and with a slight abuse of notation, we use the symbol $d\theta$ to denote the volume form of our (non-standard) spherical metric. In the sequel all the integrals will be computed with respect to this volume form.

Step 2: Computing the Commutator. In order to separate the spherical and the radial variables, we set $u = \theta_n^{\frac{2s-1}{2}} v$ and multiply with $\theta_n^{\frac{2s-1}{2}}$. Although the function v becomes increasingly singular (if $s > \frac{1}{2}$), this form of the equation has the advantage that the operator is symmetric and strictly separates the radial and spherical variables. Thus – up to the first order error terms originating from the first step – our equation turns into

$$\partial_t^2 - \frac{(n-2s)^2}{4} + \theta_n^{\frac{2s-1}{2}} \tilde{\nabla}_{S^n} \cdot \theta_n^{1-2s} \tilde{\nabla}_{S^n} \theta_n^{\frac{2s-1}{2}}.$$

Conjugation with an only t -dependent weight, ϕ , leads to the following “symmetric and antisymmetric” parts of the operator:

$$S = \partial_t^2 + \tau^2 (\partial_t \phi)^2 - \frac{(n-2s)^2}{4} + \theta_n^{\frac{2s-1}{2}} \tilde{\nabla}_{S^n} \cdot \theta_n^{1-2s} \tilde{\nabla}_{S^n} \theta_n^{\frac{2s-1}{2}},$$

$$A = -2\tau (\partial_t \phi) \partial_t - \tau \partial_t^2 \phi.$$

We point out that the ∂_t -contributions are not actually symmetric and antisymmetric with respect to our non-standard spherical metric, yet this separation of the full operator into S and A proves to be convenient for the calculations of the pairing $(Su, Au)_{L^2(S_+^n \times \mathbb{R})}$. All the occurring error terms can be controlled. If ϕ is sufficiently pseudoconvex the separation into S and A yields the following “commutator” terms:

$$4\tau^3 \left\| (\partial_t^2 \phi)^{\frac{1}{2}} \partial_t \phi v \right\|_{L^2(S_+^n \times \mathbb{R})} + 4\tau \left\| (\partial_t^2 \phi)^{\frac{1}{2}} \partial_t v \right\|_{L^2(S_+^n \times \mathbb{R})} - \tau \int_{S_+^n \times \mathbb{R}} \partial_t^4 \phi v^2 d\theta dt$$

$$+ (\text{ER}),$$

where (ER) is used to denote any bulk term involving derivatives of g which is controlled by

$$\tau \int_{S_+^n \times \mathbb{R}} |\partial_t \phi| |\tilde{\nabla} v|^2 |\nabla g| d\theta dt. \quad (3.10.2)$$

We remark that all integrals are calculated with respect to our non-standard spher-

ical metric. In these calculations one has to be slightly more careful than in the case of the standard sphere as the metric tensor, and thus the volume element, also depends on the t -variable. As a consequence, it is more convenient to calculate some of the quantities appearing in $(Su, Au)_{L^2_g(S_+^n \times \mathbb{R})}$ directly, instead of symmetrizing and antisymmetrizing the respective contributions. Contributions of the form (ER) will be treated as errors, c.f. Step 4.

Furthermore, weighted gradient estimates can be obtained:

$$\begin{aligned}
& ((\partial_t^2 \phi) \partial_t v, \partial_t v) + ((\partial_t^2 \phi) \theta_n^{1-2s} \tilde{\nabla}_{S^n} \theta_n^{-\frac{1-2s}{2}} v, \tilde{\nabla}_{S^n} \theta_n^{-\frac{1-2s}{2}} v) \\
= & - (Sv, (\partial_t^2 \phi) v) + \int_{\partial S_+^n \times \mathbb{R}} (\partial_t^2 \phi) (\theta_n^{1-2s} \nu \cdot \tilde{\nabla}_{S^n} \theta_n^{-\frac{1-2s}{2}} v) \theta_n^{-\frac{1-2s}{2}} v d\theta dt \\
& + ((\partial_t^4 \phi) v, v) + (\text{ER}) \\
\leq & \frac{1}{2\tau^2} \|Sv\|_{L^2}^2 + \frac{\tau^2}{2} \|(\partial_t^2 \phi) v\|_{L^2}^2 + \tau^2 \left\| (\partial_t^2 \phi)^{\frac{1}{2}} \partial_t \phi v \right\|_{L^2}^2 - \frac{(n-2)^2}{4} \left\| (\partial_t^2 \phi)^{\frac{1}{2}} v \right\|_{L^2}^2 \\
& + \int_{\partial S_+^n \times \mathbb{R}} (\partial_t^2 \phi) (\theta_n^{1-2s} \nu \cdot \tilde{\nabla}_{S^n} \theta_n^{-\frac{1-2s}{2}} v) \theta_n^{-\frac{1-2s}{2}} v d\theta dt \\
& + ((\partial_t^4 \phi) v, v) + (\text{ER}),
\end{aligned} \tag{3.10.3}$$

where $\nu = (0, \dots, 0, -1)$ denotes the outer unit normal. For sufficiently pseudoconvex weight, ϕ , the right hand side can even be controlled via the commutator contributions if everything is multiplied by a factor of $c\tau$, for example $c \sim \frac{1}{2}$ would work. The boundary integral can be evaluated to yield

$$\begin{aligned}
& \int_{\partial S_+^n \times \mathbb{R}} (\partial_t^2 \phi) (\theta_n^{1-2s} \nu \cdot \tilde{\nabla}_{S^n} \theta_n^{-\frac{1-2s}{2}} v) \theta_n^{-\frac{1-2s}{2}} v d\theta dt \\
& = \int_{\partial S_+^n \times \mathbb{R}} \theta_n^{-(1-2s)} (\partial_t^2 \phi) e^{2st} V v^2 d\theta dt,
\end{aligned}$$

where by a slight abuse of notation we also denote the lower dimensional volume form by $d\theta dt$. We note that the gradient contribution in (3.10.3) (multiplied with τ) in particular suffices to absorb the bulk contribution of (3.10.2).

The remaining boundary integral which originates from the commutator calculation

is given by

$$\begin{aligned}
& 4\tau \int_{\partial S_+^n \times \mathbb{R}} (\theta_n^{1-2s} \nu \cdot \tilde{\nabla}_{S^n} \theta_n^{-\frac{1-2s}{2}} v) (\partial_t \phi) \theta_n^{-\frac{1-2s}{2}} \partial_t v d\theta dt + (\text{BER}) \\
& + 2\tau \int_{\partial S_+^n \times \mathbb{R}} (\theta_n^{1-2s} \nu \cdot \tilde{\nabla}_{S^n} \theta_n^{-\frac{1-2s}{2}} v) (\partial_t^2 \phi) \theta_n^{-\frac{1-2s}{2}} v d\theta dt \\
& = 4\tau \int_{\partial S_+^n \times \mathbb{R}} (\partial_t \phi) \theta_n^{-(1-2s)} e^{2st} V v \partial_t v d\theta dt \\
& + 2\tau \int_{\partial S_+^n \times \mathbb{R}} (\partial_t^2 \phi) \theta_n^{-(1-2s)} e^{2st} V v^2 d\theta dt + (\text{BER}),
\end{aligned}$$

where (BER) denotes boundary contributions involving derivatives of the metric, e.g. terms bounded by $\tau \int_{\partial S_+^n \times \mathbb{R}} |\partial_t \phi \partial_t \bar{g} e^{2st} V| u^2 d\theta dt$. Rewritten in terms of $u = \theta_n^{-\frac{1-2s}{2}} v$ the Carleman estimate reads

$$\begin{aligned}
& c\tau \left\| (\partial_t^2 \phi)^{\frac{1}{2}} \theta_n^{\frac{1-2s}{2}} \partial_t u \right\|_{L^2}^2 + c\tau \left\| (\partial_t^2 \phi)^{\frac{1}{2}} \theta_n^{\frac{1-2s}{2}} \tilde{\nabla}_{S^n} u \right\|_{L^2}^2 \\
& + c\tau^3 \left\| \theta_n^{\frac{1-2s}{2}} (\partial_t^2 \phi)^{\frac{1}{2}} (\partial_t \phi) u \right\|_{L^2}^2 \\
& + \left\| S(\theta_n^{\frac{1-2s}{2}} u) \right\|_{L^2}^2 + \tau^{-1} \left\| (\partial_t^2 + \theta_n^{-\frac{1-2s}{2}} \tilde{\nabla}_{S^n} \cdot \theta_n^{1-2s} \tilde{\nabla}_{S^n} \theta_n^{-\frac{1-2s}{2}}) \theta_n^{\frac{1-2s}{2}} u \right\|_{L^2}^2 \\
& + 4\tau \int_{\partial S_+^n \times \mathbb{R}} (\partial_t \phi) e^{2st} V u \partial_t u d\theta dt + 2\tau \int_{\partial S_+^n \times \mathbb{R}} (\partial_t^2 \phi) e^{2st} V u^2 d\theta dt \\
& + c\tau \int_{\partial S_+^n \times \mathbb{R}} (\partial_t^2 \phi) e^{2st} V u^2 d\theta dt + (\text{BER}) \\
& \leq \|L_\phi u\|_{L^2}^2,
\end{aligned} \tag{3.10.4}$$

where

$$\begin{aligned}
L_\phi &= \theta_n^{\frac{1-2s}{2}} (\partial_t^2 + \tau^2 (\partial_t \phi)^2) - \frac{(n-2s)^2}{4} - 2\tau (\partial_t \phi) \partial_t - \tau \partial_t^2 \phi \\
& + \theta_n^{\frac{2s-1}{2}} \tilde{\nabla}_{S^n} \cdot \theta_n^{1-2s} \tilde{\nabla}_{S^n}.
\end{aligned}$$

It remains to discuss the unsigned boundary contributions and the error terms.

Step 3: Bounding the Boundary Contributions. In order to estimate the unsigned boundary contributions from the previous steps, we consider the respective expressions in polar coordinates as in (3.10.4). Starting with the scaling-critical potentials,

we have to bound

$$\begin{aligned} & 4\tau \int_{\partial S_+^n \times \mathbb{R}} (\partial_t \phi) e^{2st} V_1 u \partial_t u d\theta dt + 2\tau \int_{\partial S_+^n \times \mathbb{R}} (\partial_t^2 \phi) e^{2st} V_1 u^2 d\theta dt \\ & + c\tau \int_{\partial S_+^n \times \mathbb{R}} (\partial_t^2 \phi) e^{2st} V_1 u^2 d\theta dt + \tau \int_{\partial S_+^n \times \mathbb{R}} |\partial_t \phi (\partial_t g) e^{2st} V_1| u^2 d\theta dt, \end{aligned}$$

i.e. we have to control the boundary integrals involving the potential $V_1 = e^{-2st} h(\theta)$. By an integration by parts in t , we obtain that most contributions drop out. Indeed, the conditions on a imply that the only non-vanishing terms can be estimated by $C\tau \int_{\partial S_+^n \times \mathbb{R}} |\partial_t^2 \phi| |h(\theta)| u^2 d\theta dt$. However, by appealing to the interpolation inequality (3.6.3), this can be controlled by the positive quantities of the Carleman inequality:

$$\begin{aligned} \tau \int_{\partial S_+^n \times \mathbb{R}} (\partial_t^2 \phi) u^2 d\theta dt & \leq \tau^{1-2s} \left\| (\partial_t^2 \phi)^{\frac{1}{2}} \theta_n^{\frac{1-2s}{2}} \nabla u \right\|_{L^2(S_+^n \times \mathbb{R})}^2 \\ & + \tau^{3-2s} \left\| (\partial_t^2 \phi)^{\frac{1}{2}} \theta_n^{\frac{1-2s}{2}} u \right\|_{L^2(S_+^n \times \mathbb{R})}^2, \end{aligned}$$

where $\nabla = (\partial_t, \tilde{\nabla}_{S^n})$. Here we also used the explicit expression of ϕ and the support condition on u .

All the remaining boundary contributions involve the potential V_2 which has subcritical growth at zero. Due to the form of ϕ , it suffices to deduce control of the term

$$4\tau \int_{\partial S_+^n \times \mathbb{R}} (\partial_t \phi) e^{2st} V_2 u \partial_t u d\theta dt.$$

Integrating by parts in t , using the subcriticality of V_2 and the properties of ϕ and a , it suffices to bound

$$C\tau \int_{\partial S_+^n \times \mathbb{R}} e^{\epsilon t} u^2 d\theta dt.$$

Again, this can be controlled by the interpolation inequality (3.6.3).

Step 4: Treatment of the Error Contributions. It remains to comment on the first order error terms from step 1 and from the conjugation process. The terms from step 1 also undergo the conjugation process. Under this they either remain unchanged or involve a derivative of ϕ and a prefactor of τ . Instead of including these contributions – which, in the following, we denote by (Er) – in the commutator calculation, we treat them as errors:

$$\|e^{\tau\phi} Lw\|_{L^2} = \|(S + A + Er)u\|_{L^2} \geq \|(S + A)u\|_{L^2} - \|(Er)u\|_{L^2}.$$

Due to the assumptions on a and the fact that these terms are only of first order, it is possible to absorb these specific errors – as well as any error terms of the form (ER) – into the positive commutator contributions which were deduced in step 3. \square

Combined with a blow-up procedure comparable to the one carried out in Section 3.7.2, the strong unique continuation property follows. As the blown-up solution satisfies an equation with *constant* coefficients, the strong unique continuation result can be regarded as a consequence of a weak unique continuation statement of the same flavour as the one presented in Section 3.5.

3.10.2 Carleman Inequalities in the Case of Non-Flat Domains

The previous discussion of the situation in \mathbb{R}_+^{n+1} illustrates that it is possible to deal with our (degenerate) elliptic operators if they are defined on a manifold of the form $(\mathbb{R}_+ \times M, 1 \times g_{ij})$. Here (M, g_{ij}) is a Riemannian manifold which has – in a Lipschitz sense – a metric which is sufficiently close to a constant non-degenerate metric. In particular, this allows to deal with operators of the form (3.10.1) – i.e. operators in which there is a clear distinction between normal and tangential variables, as, sufficiently close to the boundary, an appropriate choice of normal coordinates allows to cast the equation into (a lower order perturbation of) the previously discussed setting of \mathbb{R}_+^{n+1} .

3.10.3 Comments on the Situation with a Spectral Gap

In settings involving a spectral gap, the situation improves significantly. In fact, under these assumptions it is possible to argue as in the article of Koch and Tataru [KT01a] in which a radial summability condition is required – which is based on stronger estimates originating from a spectral gap condition. Thus, in situations involving a spectral gap, it is possible to control equations with leading order contributions of the form $\partial_i y_{n+1}^{1-2s} g_{ij}(y) \partial_j$ and bounds of the type $|y| |\nabla g| \in l^1(L^\infty)$, c.f. [KT01a].

Part II

The Cubic-to-Orthorhombic Phase Transition

Chapter 4

Introduction

Shape-Memory Materials

Shape-memory materials are metal alloys which undergo a diffusionless, temperature- or stress-induced solid-solid phase transition with a single, highly symmetric high temperature state – the so-called austenite – and various less symmetric low temperature states – the different variants of martensite. This variety of low temperature states is reflected in a great flexibility of shape-memory materials at low temperatures: A sample of a shape-memory alloy can, for example, be deformed into very different shapes with comparably little energetical effort in the low temperature regime. On heating this deformed material above its (material-specific) critical temperature, the atoms are forced back into their original, highly symmetric lattice. As a consequence, the deformation is “undone”; the material “remembers” its original shape – it displays the shape-memory effect [Bha03].

As is easily conceivable, such materials are very promising for various industrial applications as they can be produced to “remember” their high temperature shape which is a desirable property for certain applications. For example, this can be exploited in transporting bulky devices efficiently: Instead of directly transporting the device to the position at which it is needed, it can be more efficient to first transform it into a less bulky transportation shape. For shape-memory alloys this can be achieved by cooling the material into its martensitic phase and then deforming it at very low energy cost. On reaching the place at which the shape-memory device is needed, a temperature- or stress-induced phase transformation can then return the material into its original, high temperature form. Applications of this are, for example, essential in aeronautics (e.g. for sun collectors of satellites) or medicine (e.g. stents which are introduced into the body, braces etc.). Further applications are feasible.

Such materials, however, are not only interesting from an engineering or physical point of view but also deserve an intensive investigation due to the challenging mathematical features of the associated models describing them. In this context the

modeling of material properties imposes conditions which cannot be treated with the “standard” tools of convex variational analysis. In describing these materials (in a static situation) within a continuum theory, there are essentially two approaches from a mathematical point of view:

- **Differential Inclusions.** On the one hand, the stress-free strains of a material can be explicitly measured. On the other hand, the Hamiltonian determining the material behaviour is, in general, not known. Therefore, it is attractive to consider only the stress-free states as assumptions of the model, while not requiring additional physical input. This leads to a so-called m -well problem. In the linear theory of elasticity it reads

$$e(\nabla u) = \frac{1}{2}(\nabla u + \nabla^t u) \in \{e_1, \dots, e_m\}. \quad (4.0.1)$$

Thus, without asking for further physical assumptions, the possible (exactly stress-free) material configurations can be analyzed. This approach has been pursued by various authors (both in the linear and nonlinear settings), c.f. [DM95b], [DM95a], [Kir98], [CDK07].

- **(Non-convex) Energy Functionals.** Working more quantitatively (which might for example be necessary if one does not only consider exact solutions of the differential inclusion but also configurations which deviate from the stress-free solutions by a small amount), it becomes necessary to model a (continuum) Hamiltonian. As this has to reflect both the material invariances and the frame indifference, it is impossible to work with convex or quasiconvex integrands. This implies that certain tools originating from the direct method of the calculus of variations cannot be applied directly – for example, the functionals are no longer lower semicontinuous in general. This is reflected in a variety of minimizing sequences which depict different material patterns. Introducing surface energy, i.e. higher order regularizing energy contributions, these microstructures can be used to predict the material behaviour [DM95a], [CO12].

A related approach (which is a possible relaxation of non-quasiconvex integrands) consists of avoiding the lack of weak lower semicontinuity in the functionals by working in weaker spaces, in general in measure spaces. Here the notion of “Young measures” provides a very strong tool in understanding (oscillation) properties of the microstructures (in the absence of surface energy contributions) [Ped97], [Bal89], [KP91].

Although the previous distinction is very crude – in the treatment of both of these directions various different methods evolved which can be used to tackle the respective problems – it depicts the basic choice in the modeling of shape-memory alloys (in a static regime).

The Results of the Thesis

In the sequel we investigate a specific martensitic phase transition – the so-called cubic-to-orthorhombic phase transition (c.f. below for the details of the model). Here a cubic lattice is deformed into an orthorhombic one at the critical temperature. The industrially most important material undergoing this transition is CuAlNi. This material is of particular interest as physical experiments suggest that it displays a large variety of microstructures, i.e. it is very flexible in its low temperature phase.

In the present work we mathematically investigate the six-well problem as a differential inclusion describing the (exactly stress-free) material (in its low temperature phase). In this setting we obtain two main results:

- **Non-Rigidity.** Investigating the six-well problem in the linear theory of elasticity, we observe a mathematically very interesting, but physically unexpected behaviour: There is a rich variety of very “wild” solutions, which are mathematically correct but which have to be rejected on physical grounds (they do not depict any type of characteristic length scale). This phenomenon indicates that the pure six-well problem does not fully capture the physical features of the cubic-to-orthorhombic phase transition. Similar observations were previously made in the context of *nonlinear* models [DM95b], [DKMŠ00a], [CDK07]. In a sense, our phase transition describes one of the simplest three-dimensional, physically relevant settings in which already the *linear* theory exhibits very “wild”, non-rigid solutions. This is presented in Chapter 5.
- **Rigidity.** The previously described “physical ill-posedness result” is complemented by a rigidity result in the case of additional surface energy control. As the non-rigidity properties are consequences of highly irregular phase distributions, a natural strategy to rule these out consists of introducing higher order regularizing constraints. Here, we use the “most primitive” version of surface energy by restricting to piecewise polygonal configurations, i.e. configurations for which the support of each phase consists of an arbitrary but finite number of disjoint, piecewise polygonal domains. For these configurations we prove rigidity: Instead of the very wild convex integration configurations, we identify twin and crossing twin patterns as the generic configurations if surface energy contributions are included in the model (c.f. Chapter 6 and Figure 4.3).

Experimentally observed configurations, however, are, in general, neither given by piecewise polygonal nor only by the exactly stress-free configurations but also include those which are nearly stress-free in an energetic sense. Hence, natural further questions/topics are

- **Rigidity under BV conditions.** A natural question to pose, is whether the rigidity result which is proved in the setting of piecewise polygonal configurations remains true under “milder” surface energy constraints. The existing

literature suggests that imposing BV conditions should be the right framework to provide rigidity. However, it seems as if this were not tractable with the presented methods.

- **Energy Quantification.** An extremely interesting issue in eventually understanding the structure of microstructures would be a rigorous quantification of the energy scaling of the phase transition. As in the seminal paper of Kohn and Müller [KM94], this would provide hints on the optimal shape of the emerging patterns. Analogous to the work of Conti [Con00], this could be a starting point for a more refined analysis of the microstructures.

An energy quantification in the spirit of the articles by Capella and Otto [CO09], [CO12] has been carried out in a simplified version of the cubic-to-orthorhombic phase transition in [Rül10] (however, this simplified model excludes convex integration solutions in the stress-free setting). It remains an outstanding challenge to carry this out for the full model. In particular, it would be extremely interesting to analyze how the existence of convex integration solutions is reflected in the scaling of the energy, c.f. [Bal02].

These and related questions are possible directions of future research.

4.1 The Model

The cubic-to-orthorhombic phase transition is an important example of a solid-solid, diffusionless, temperature- or stress-induced phase transition. In its face-to-body centered transition it describes the deformation of a highly symmetric cubic lattice into a less symmetric orthorhombic one (c.f. [Bha03] for further information).

Derivation of the Strain Matrices

Thinking of the phase transition as a deformation of the underlying atomic lattice, a martensitic solid-solid phase transition can be described by its respective transition matrices or bain strains. In the face-to-body centered cubic-to-orthorhombic phase transition (c.f. Figure 4.1) this amounts to the following linear deformation

$$\frac{a_0}{\sqrt{2}} \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix} \mapsto c \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}, \quad \frac{a_0}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \mapsto a \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \quad a_0 \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \mapsto b \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}.$$

Rewriting this in terms of the austenitic basis leads to the following transition matrix

$$U = \begin{pmatrix} \frac{\alpha+\gamma}{2} & 0 & \frac{\alpha-\gamma}{2} \\ 0 & \beta & 0 \\ \frac{\alpha-\gamma}{2} & 0 & \frac{\alpha+\gamma}{2} \end{pmatrix},$$

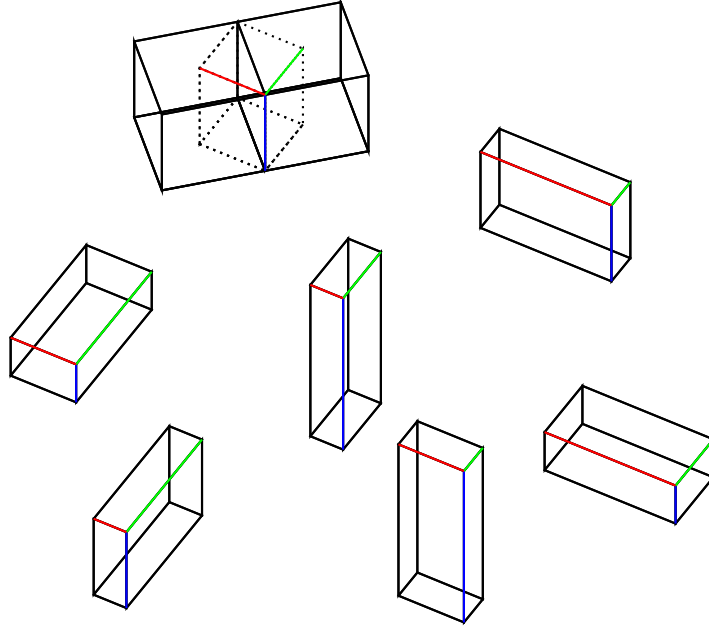


Figure 4.1: The transformation from the cubic austenite lattice to the low temperature lattices associated with the different variants of martensite. The austenite lattice is cubic (top). The martensite lattices are obtained by stretching and compressing along a given edge of the austenite lattice and associated face diagonals. This leads to the six (symmetry related) variants of martensite (bottom).

where $\alpha = \frac{\sqrt{2}a}{a_0}$, $\beta = \frac{b}{a_0}$, $\gamma = \frac{\sqrt{2}c}{a_0}$. In CuAlNi, these parameters are of the order $a_0 = 5.8 \text{ \AA}$, $a = 4.38 \text{ \AA}$, $b = 5.36 \text{ \AA}$, $c = 4.22 \text{ \AA}$, c.f. [Bha03]. Taking into account the symmetry of the cubic and the orthorhombic lattices, implies that there are five further strain matrices. Indeed, for a fixed parameter b it is always possible to exchange the roles of a and c . Moreover, it is also possible to permute the austenitic basis vectors. As a consequence, the phase transition is characterized by the following six transformation matrices

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

Cauchy-Born Hypothesis and Linearization

The previously derived discrete model is now linked to a continuum model via the *Cauchy-Born hypothesis*. This assumes that microscopically the atomic lattice is deformed according to the macroscopic deformation $F(x)$. More precisely, if a macroscopic deformation at a point x is given by $F(x)$, we assume that a local microscopic lattice spanned by the vectors $\{v_1(x), v_2(x), v_3(x)\}$ is deformed accordingly, yielding a new lattice $\{F(x)v_1(x), F(x)v_2(x), F(x)v_3(x)\}$. Under certain assumptions this rule can be rigorously verified, c.f. [Eri08], [CDKM05], [WnPb07]. Although it does not hold true in general, we will make this assumption in the sequel. Hence, it is heuristically justified to assume that a stress-free macroscopic deformation is described by the transformation matrices U_1, \dots, U_6 .

However, these are not all possible stress-free states. Apart from the invariance dictated by the material – which gives rise to the different martensitic wells in the first place – a second symmetry has to be taken into consideration. The model has to be frame indifferent. As a consequence, the set of stress-free deformation matrices is given by

$$\nabla u \in \bigcup_{j=1}^6 SO(3)U_j.$$

This leads to a so-called six-well problem. In this model there are two sources of nonlinearity: On the one hand, the material symmetry leads to six possible martensitic variants. On the other hand, the frame indifference creates an additional geometric nonlinearity in matrix-space by imposing $SO(3)$ invariance.

In order to avoid this second nonlinearity we adopt a geometrically linear point of view. Formally linearizing (around the identity) leads to

$$\nabla u \in \{e^{(1)}, \dots, e^{(6)}\} + Skew,$$

or, written as a differential inclusion for the symmetrized gradient,

$$e(\nabla u) = \frac{1}{2}(\nabla u + \nabla^t u) \in \{e^{(1)}, \dots, e^{(6)}\},$$

as the skew symmetric matrices are the linearization of $SO(n)$ at the identity and $e^{(i)} = U_i - Id$. Rescaling and concentrating on (infinitesimally) volume preserving transformations, we adopt the following notation

$$\begin{aligned} e^{(1)} &= \epsilon \begin{pmatrix} 1 & \delta & 0 \\ \delta & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}, & e^{(2)} &= \epsilon \begin{pmatrix} 1 & -\delta & 0 \\ -\delta & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}, & e^{(3)} &= \epsilon \begin{pmatrix} 1 & 0 & \delta \\ 0 & -2 & 0 \\ \delta & 0 & 1 \end{pmatrix}, \\ e^{(4)} &= \epsilon \begin{pmatrix} 1 & 0 & -\delta \\ 0 & -2 & 0 \\ -\delta & 0 & 1 \end{pmatrix}, & e^{(5)} &= \epsilon \begin{pmatrix} -2 & 0 & 0 \\ 0 & 1 & \delta \\ 0 & \delta & 1 \end{pmatrix}, & e^{(6)} &= \epsilon \begin{pmatrix} -2 & 0 & 0 \\ 0 & 1 & -\delta \\ 0 & -\delta & 1 \end{pmatrix}, \end{aligned}$$

where ϵ and δ are the remaining (dimensionless) material parameters. As a consequence of the linearization procedure, the material symmetry remains the only source of nonlinearity in the resulting six-well problem. This allows to study the problem from a mathematically simpler point of view while still preserving the model's main physical feature. However, one has to keep in mind, that linearized models of elasticity can provide very accurate predictions in certain situations but can also lead to major discrepancies with the corresponding nonlinear models (c.f. the discussion in [Bha93] and [Bha03]). In our situation we expect to obtain qualitatively accurate results while the precise quantitative behaviour of the material is certainly not captured.

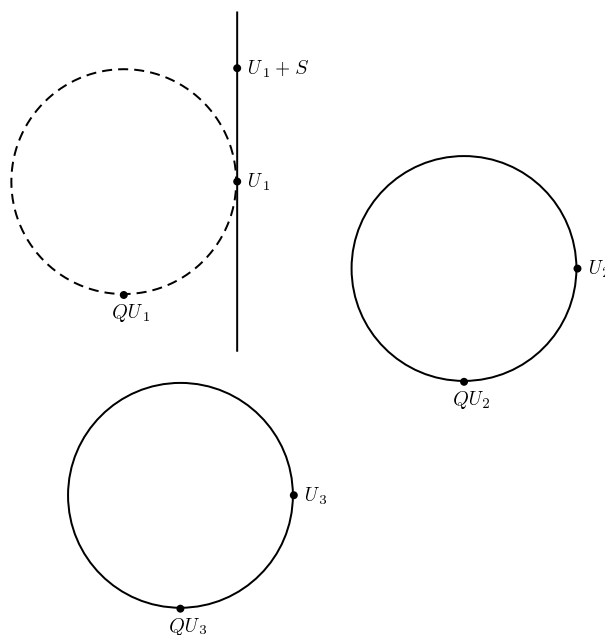


Figure 4.2: The nonlinear and linearized energy wells.

4.2 Heuristics

In this section we discuss properties of the previously derived model for the cubic-to-orthorhombic phase transition. In particular, we describe compatible piecewise affine constructions.

Symmetrized Rank-One-Connections

Motivated by classifying possible stress-free patterns which occur in the cubic-to-orthorhombic phase transition, we remark that any pair of strains is (symmetrized) rank-one-connected (c.f. Table 4.1), i.e. there exist (up to permutation) unique

$e^{(j_1)}$	$e^{(j_2)}$	normals	$e^{(j_1)}$	$e^{(j_2)}$	normals
$e^{(1)}$	$e^{(2)}$	$[1, 0, 0], [0, 1, 0]$	$e^{(2)}$	$e^{(6)}$	$[1, 0, -1], [3, -2\delta, 3]$
$e^{(1)}$	$e^{(3)}$	$[0, 1, -1], [2\delta, 3, 3]$	$e^{(3)}$	$e^{(4)}$	$[1, 0, 0], [0, 0, 1]$
$e^{(1)}$	$e^{(4)}$	$[0, 1, 1], [2\delta, 3, -3]$	$e^{(3)}$	$e^{(5)}$	$[1, -1, 0], [3, 3, 2\delta]$
$e^{(1)}$	$e^{(5)}$	$[1, 0, -1], [3, 2\delta, 3]$	$e^{(3)}$	$e^{(6)}$	$[1, 1, 0], [3, -3, 2\delta]$
$e^{(1)}$	$e^{(6)}$	$[1, 0, 1], [3, 2\delta, -3]$	$e^{(4)}$	$e^{(5)}$	$[1, 1, 0], [-3, 3, 2\delta]$
$e^{(2)}$	$e^{(3)}$	$[0, 1, 1], [2\delta, -3, 3]$	$e^{(4)}$	$e^{(6)}$	$[1, -1, 0], [3, 3, -2\delta]$
$e^{(2)}$	$e^{(4)}$	$[0, 1, -1], [-2\delta, 3, 3]$	$e^{(5)}$	$e^{(6)}$	$[0, 1, 0], [0, 0, 1]$
$e^{(2)}$	$e^{(5)}$	$[1, 0, 1], [-3, 2\delta, 3]$			

Table 4.1: Pairs of strains with their respective (symmetrized, not normalized) rank-one-connections.

vectors $n_{ij} \in \mathbb{S}^2$, $a_{ij} \in \mathbb{R}^3 \setminus \{0\}$ such that

$$e^{(i)} - e^{(j)} = \frac{1}{2}(a_{ij} \otimes n_{ij} + n_{ij} \otimes a_{ij}) \text{ if } i \neq j. \quad (4.2.1)$$

From this we deduce that any pair of strains can form laminates/ twin configurations, i.e. there exists a vector field $u : \mathbb{R}^3 \rightarrow \mathbb{R}^3$, $u \in W^{1,\infty}$, and a plane determined by one of the vectors n_{ij} (or a_{ij}) such that $e(\nabla u) = e^{(i)}$ for $x \cdot n_{ij} \geq 0$ and $e(\nabla u) = e^{(j)}$ for $x \cdot n_{ij} < 0$ (c.f. Figure 4.3, (b)). This is a result of tangential continuity.

We remark that, as all matrices $e^{(j)}$ are tracefree, the vectors a_{ij} and n_{ij} are orthogonal: $a_{ij} \cdot n_{ij} = 0$. We further point out that the respective normals n_{ij} , a_{ij} include vectors with and without δ entries (up to normalization). While the ones without δ entries occur exactly twice as the normals between two pairs of distinct strains, the vectors involving δ entries can be uniquely associated with a single pair of strains (up to permutation). In the case of $\delta = 0$ the rank-one connections collapse to those of the cubic-to-tetragonal phase transition.

Corners of Higher Degree

Experiments suggest that apart from simple laminates the cubic-to-orthorhombic phase transition also allows for so-called crossing twin constructions. These are configurations in which two distinct pairs of twins meet at a given plane. At this plane necessarily corners consisting of three or four strains are involved. As a consequence, it is desirable to develop an understanding of conditions allowing for such corners of higher degree. Due to the necessary tangential continuity at the jump interfaces, the twinning condition (4.2.1) imposes a necessary condition. However, it does not provide a sufficient condition as in the case of three or more strains an additional condition is needed in order to ensure the compatibility of the skew symmetric parts of the vector field u . If a corner is constituted of the strains A_1, \dots, A_n satisfying

$$A_j - A_{j+1} = \frac{1}{2}(a_j \otimes n_j + n_j \otimes a_j) \text{ for } j \in \{1, \dots, n\},$$

the compatibility of the skew symmetric part is equivalent to

$$\sum_{j=1}^n a_j \otimes n_j = 0. \quad (4.2.2)$$

Computing this condition for the cubic-to-orthorhombic phase transition for arbitrary combinations of four strain variants, leads to the observation that for specific combinations of the strain matrices such corners exist and can be combined to yield crossing twin constructions (as predicted by the experimental results), c.f. Figure 4.3, (a) and Figures 6.4, 6.5 and 6.6 in Chapter 6 for further crossing twin configurations.

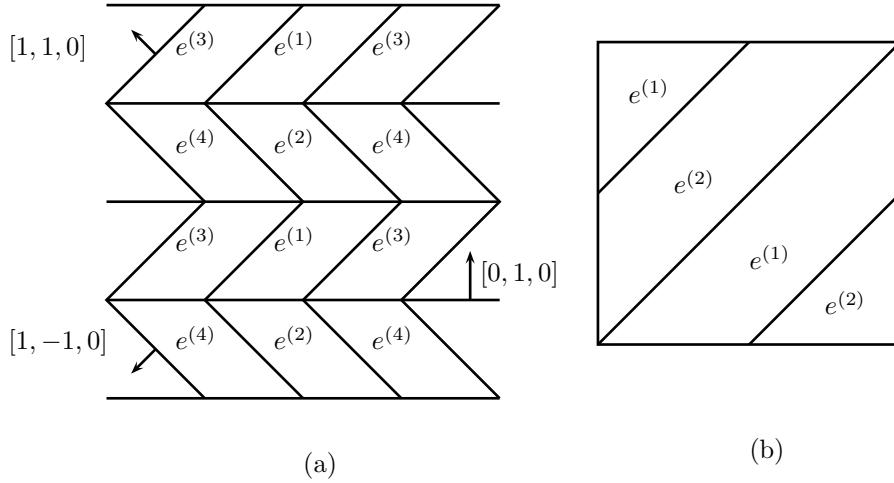


Figure 4.3: Examples of (a) crossing twin structures, (b) laminate structures. The crossing twin structures are built up of two pairs of twins: There is an “outer structure” determined by the common jump plane of the twinning pairs (in our picture these are the planes with normal $[0, 1, 0]$) as well as an “inner structure” made up of “zig-zag bands” of twins (in our picture these are the twinning bands given by $e^{(4)} - e^{(3)}$ and $e^{(2)} - e^{(1)}$, respectively).

Compatible Microstructures

The cubic-to-orthorhombic phase transition allows for a variety of microstructures: Apart from the exactly compatible configurations described above, it is possible to accommodate any boundary condition whose symmetrized gradient lies in the convex hull of the strains [Bha03], [BK97] (in the geometrically linear situation). This corresponds to the fact that the quasiconvex hull of the strains agrees with the convex hull, i.e. it is very large. Moreover, (in the geometrically linear setting) any convexification of the strains coincides with the convex hull of the strains:

$$\{e^{(1)}, \dots, e^{(6)}\}^{lc} = \{e^{(1)}, \dots, e^{(6)}\}^{co}.$$

Although it is a very interesting and challenging topic to determine the “energetically most efficient” microstructures corresponding to certain boundary conditions, we do not pursue this any further in the sequel. We only remark that such an investigation would be the natural next step after analyzing all exactly stress-free patterns, as microstructures can usually accommodate a much larger variety of boundary conditions than exactly stress-free patterns and as these are usually the physically observed states of the material. Such an analysis has been carried out for a simplified model of the cubic-to-orthorhombic phase transition in [Rül10]. The energetic scaling analysis of the full model would be of particular interest – not only from a physical point of view but also from a mathematical viewpoint as it would indicate whether the “wild” convex integration solutions are “seen” in an energetically quantified model. John Ball has rated this open issue as one of the most fascinating and challenging problems in elasticity, c.f. [Bal02], Problem 17. Although there are some promising attempts pointing to an improved understanding of this problem (c.f. [Cha13]), it remains an outstanding challenge in the mathematical theory of elasticity/ shape-memory alloys.

Chapter 5

Non-Rigidity

5.1 Introduction

This first part dedicated to the cubic-to-orthorhombic phase transition can be viewed from two perspectives: On the one hand, it deals with the (meta-) question of whether the described pure six-well problem can be considered a “physically correct” model for the cubic-to-orthorhombic phase transition. On the other hand, it is a mathematical investigation of solutions of the differential inclusion problem associated with this phase transition.

In experiments a variety of different microstructures are observed for this phase transition. However, none of them is “too wild” (in the sense that only very characteristic patterns occur). In the sequel we will show that our first mathematical model which is given by the differential inclusion (4.0.1) does not reflect this feature. In a sense, it admits “too many” exactly stress-free solutions. Mathematically, this is a consequence of the method of convex integration as crucially developed by Müller and Šverák [MŠ99].

Convex Integration and Elasticity

Convex integration is a technique which was first introduced by Nash and Kuiper in their seminal papers on the rigidity of isometric immersions, c.f. [Nas54], [Kui55]. Using this technique they demonstrate that C^1 isometric embeddings of the sphere S^2 (into \mathbb{R}^3) are not only given by rigid motions as in the case of C^2 isometric immersions but allow for much greater flexibility. Effectively this is achieved by sophisticatedly introducing high oscillations, c.f. [Nas54], [Kui55], [Gro73], [Spr98], [CDLSJ12], [SJ13]. This idea was systematically extended by Gromov [Gro73] who applied these methods to general differential inclusions. In the following decades the techniques were developed further by authors such as Dacorogna [DM95b], [Dac07] and Müller & Šverák [MŠ99], [MŠ98]. While the first school emphasized the ideas of the Baire category approach, the second developed the method of convex integration based on in-approximations. Later these approaches were unified in the work

of Kirchheim [Kir98].

Both approaches were in part driven by the aim of improving the understanding of certain martensitic phase transitions. The relevance of these techniques to (mathematical) material scientists is highlighted by John Ball referring to the investigation of the m -well problem as the 17th problem in his personal choice of the most interesting open tasks in elasticity [Bal02]. For certain phase transitions this problem has been solved. In the sequel we review a few contributions to this field. Again, this selection is rather crude. It excludes important facets, but is intended to display characteristic properties of certain models of phase transitions which are comparable to our setting.

- **The Two-Well Problem.** The (two-dimensional) two-well problem deals with the following inclusion problem:

$$\begin{aligned} \nabla u &\in SO(2)U_0 \cup SO(2)U_1, \det(U_0), \det(U_1) > 0 \\ \text{or } \nabla u &\in \{E_0, E_1\} + Skew(2) \end{aligned}$$

in the nonlinear and in the linear situations, respectively.

While the *linear* theory predicts a very rigid picture – locally any configuration consists of simple laminates – the *nonlinear* model does not reflect this. On the contrary, in their seminal paper Müller and Šverák [MŠ99] prove that (in the presence of rank-one connections) there are extremely many, extremely wild solutions to this problem. In order to do so, they extend the theory of Gromov in two directions: On the one hand, they work with a nonlinear codimension one inclusion problem (this is a necessary precondition in order to deal with the volume preserving two-well problem). On the other hand, they extend the methods to the *rank-one*-convex hull (instead of the laminar convex hull – which is not necessary for the two-well problem but, for example, for the cubic-to-monoclinic phase transition).

However, using regularizing effects, e.g. by imposing BV conditions on the deformation gradient, it is possible to recover a rigidity result also in the *nonlinear* picture [DM95b]. Thus, the additional regularity assumptions rule out the “wild” convex integration solutions.

As this model serves as a prototype for the more involved realistic phase transitions, it is particularly well understood: For instance, the explicit structure of the various convex hulls is known in two dimensions [Mül99] (however, this is no longer true in three or higher dimensions, c.f. [DKMŠ00b] – which illustrates how difficult these computations are). Moreover, in the linear situation even the energy scaling of the model can be described – yielding the same results as the scalar models introduced by Kohn & Müller [KM94] (in most cases), c.f. also [Con00], [Cha13]. In the nonlinear situation this seems to be a much more subtle challenge as the role of the convex integration solutions is not clear yet. However, first successful approaches to tackle parts of the problem have recently been developed in [Cha13].

- **The Cubic-to-Tetragonal Phase Transition.** This problem deals with a three-well differential inclusion of the form

$$\nabla u \in \bigcup_{i=1}^3 SO(3)(\lambda^2 e_i \otimes e_i + \frac{1}{\lambda}(Id - e_i \otimes e_i))$$

$$\text{or } \nabla u \in \bigcup_{i=1}^3 (-\frac{1}{2}Id + \frac{3}{2}e_i \otimes e_i) + Skew,$$

in its nonlinear and linear versions. This represents one of the simplest (realistic) martensitic phase transitions (which, however, is highly nontrivial from a mathematical point of view). As in the two-well problem the *linear* theory predicts rigidity: In [DM95a], Dolzmann and Müller prove that locally the only compatible, stress-free patterns consist of simple laminates with normals dictated by the associated rank-one conditions. Again, the *nonlinear* differential inclusion does not exhibit this behaviour: Convex integration solutions can be shown to exist [CDK07]. Due to the non-commutativity of $SO(3)$, it is not possible to transfer the methods of the nonlinear, BV constrained rigidity result of Müller & Dolzmann [DM95b] into the three-dimensional setting. Yet, in [Kir98] Kirchheim shows that the statement still holds true in spite of the described difficulties. Using strongly combinatorial elements which are specific to the cubic-to-tetragonal phase transition, he proves rigidity under BV assumptions.

For this phase transition not all the convex hulls are known explicitly: While the linear theory states that

$$\{e_1, e_2, e_3\}^{lc} = \{e_1, e_2, e_3\}^{co},$$

the nonlinear picture is not as clear [Bal02], [CDK07].

As in the two-well problem the scaling of the linear, energetically quantified model is fully understood, c.f. [CO09], [CO12]: Capella and Otto prove that the scaling corresponds to that of the scalar Kohn-Müller model. Even nucleation problems [KKO13] can be treated in the linear framework. However, again, the nonlinear problem poses much greater difficulties. It is not clear what to expect in that situation.

- **The Cubic-to-Orthorhombic Phase Transition.** For the cubic-to-orthorhombic phase transition several properties are known: As in the cubic-to-tetragonal phase transition, all its convex hulls coincide with the standard convex hull in the setting of the linear theory of elasticity. Experimentally, a large number of microstructures is observed. In particular, the exactly stress-free setting already allows for more complex solutions than the cubic-to-tetragonal phase transition – so-called crossing twin structures emerge, c.f. [Bha03]. In [Rül10], the author considered a simplified model for the cubic-to-orthorhombic phase transition and classified all stress-free states in

this setting. Furthermore, it was possible to prove (energetically quantified) stability of these constructions in the simplified model.

- **The Cubic-to-Monoclinic Phase Transition.** This phase transition is of particular interest, as it represents the class of the industrially most popular materials – including for instance NiTi. In the associated inclusion problem the cubic-to-monoclinic wells strictly contain the ones of the cubic-to-orthorhombic phase transition. Hence, it is plausible to expect a large number of different exactly stress-free states.

Mathematically, the cubic-to-monoclinic phase transition is particularly interesting, as it is the first phase transition for which the laminar convex hull does not coincide with the convex hull in the setting of the linear theory of elasticity (this is a consequence of the fact that not all strains are pairwise symmetrized rank-one connected). As a consequence, already the linear theory poses fascinating new questions. This phase transition has been the subject of recent research by Schlömerkemper & Chenchiah [CS12].

- **Young Measures.** A very powerful alternative approach of understanding the behaviour of the inclusion problems associated with the respective phase transitions consists of investigating the corresponding Young measures. These are measures describing the local distribution of strains/deformation in strain/matrix-space. It is an important tool in understanding oscillatory behaviour (of microstructures) and in computing the different convex hulls (via duality), c.f. [Mül99], [Ped97], [KP91], [Bha03].

Summarizing, these results create the following picture:

- In experiments configurations with “characteristic” patterns are observed. Often the materials even display rigidity in the sense that only certain patterns, e.g. simple laminates, can occur (if only small stresses are allowed).
- While the *linear* theory of elasticity often (at least in “model cases” such as the two-well problem or the cubic-to-tetragonal phase transition) predicts the “physically correct patterns”, this breaks down in the “simplest” models of the *nonlinear* theory.
- In general, the mathematical n -well models predict extremely irregular solutions which display a mixing of scales. Thus, the physical picture is not described “correctly”. A length scale has to be introduced by adding regularizing higher order terms into the model.

In this context our results provide an example of an industrially relevant phase transition which already displays non-rigidity properties in the *linear* theory of elasticity. More generally, this phenomenon can occur, if there are sufficiently many different (pairwise symmetrized rank-one connected) stress-free strains. As in the nonlinear situations in which one observes such a behaviour, the physical solutions can be separated from the unphysical ones by adding regularity constraints.

5.2 The Main Results

From a technical point of view the linearized theory of martensite differs from a gradient inclusion problem by an *unbounded* ingredient: The inclusion problem is of the form

$$\nabla u \in K + \text{Skew}(3), \quad (5.2.1)$$

where $K \subset \mathbb{R}^{3 \times 3}$ is a compact set in the tracefree matrices (which corresponds to the energy wells in the case of a phase transition). In the sequel we will investigate this inclusion problem which is slightly more general than the described six-well problem. Hence, the specific application to the six-well problem (4.0.1) will be a consequence of this discussion.

Our strategy of tackling the problem consists of keeping the unbounded ingredient, while else following the arguments of Müller and Šverák [MŠ99] in the linearized setting. Instead of using a $W^{1,\infty}$ bound, which we lack due to the unboundedness of the problem, we make use of Korn's inequality to derive slightly weaker $W^{1,p}$, $p \in (1, \infty)$, bounds. Thus, the unbounded aspects of this argument account for a loss of regularity in the final solution of the symmetrized gradient inclusion.

An alternative approach, which would yield slightly stronger non-rigid solutions (solutions in $W^{1,\infty}$) could consist of applying the ideas established by Kirchheim [Kir07]. Instead of working with the bounds obtained via Korn's inequality, one could directly “lift” the problem to a bounded differential inclusion for the gradient. In order to proceed with such a strategy, it would be necessary to identify the lamination extreme points of the lamination convex hull of the resulting set. While the situation can be handled for analogous two-dimensional problems (involving three strains, e.g. the hexagonal-to-rhombic transition) due to the low dimensionality in matrix-space, this poses greater difficulties in the three-dimensional setting. We do not pursue this idea further, but concentrate on the strategy outlined above.

In the case of the six-well problem, we observe that despite its *linear* character the inclusion problem (4.0.1) mirrors the analogous *nonlinear* situation described by Müller and Šverák [MŠ99] as well as Conti [Con08]. In fact, at first sight rather surprisingly, the three-dimensional *linear* situation needs the full strength of the technique of convex integration. This is in sharp contrast to the two-dimensional, linear hexagonal-to-rhombic phase transition. In this two-dimensional example the convex integration solutions can be constructed without the use of the oscillation control lemma – the core of the convex integration method. This is a consequence of the fact that the existence of symmetrized rank-one connections is trivial in two-dimensions.

As a result, for all the investigated inclusions central ingredients of our proofs of

the existence of “wild” convex integration solutions are

- a linearization of Conti’s construction, c.f. [Con08],
- an application of the oscillation control lemma of Müller and Šverák, c.f. [MŠ99].

In the following, we distinguish between the different convex hulls from which we choose the boundary values for the inclusion problem (5.2.1).

The Case of the Laminar Convex Hull

In the first case of interest, we consider (5.2.1) combined with boundary data, v , whose symmetrized gradient originates from the lamination convex hull of K . More precisely, v is assumed to be a piecewise affine function with $e(\nabla v) \in K^{lc}$. Although this is included in the case of $e(\nabla v) \in K^{rc}$, we discuss both cases separately, emphasizing the details in the easier situation. This can be justified by trying to avoid technical discussions as far as possible. As the case of the lamination convex hull provides the easiest setting to describe the strategy of proof (and as we are motivated by the cubic-to-orthorhombic phase transition), it is natural to discuss this case in detail. As indicated above, we interpret the gradient inclusion as an *unbounded* gradient inclusion.

As in the nonlinear setting a major difficulty of problem (5.2.1) arises from the constraint (in our situation this amounts to the vanishing trace condition), which is stable under taking the lamination convex hull (c.f. Section 5.3 for the definition and properties). Phrasing our results in analogy to Müller & Šverák [MŠ99], we define:

$$V := \{E \in \mathbb{R}_{sym}^{3 \times 3}; \operatorname{tr}(E) = 0\}.$$

With this notation our main results can be formulated. Before dealing with the actual six-well problem, we provide an existence result for differential inclusions with values in *open* sets $U \subset V$.

Proposition 21. *Let $U \subset V$ be relatively open and bounded, $\Omega \subset \mathbb{R}^3$ bounded, open, Lipschitz and assume that $v : \Omega \subset \mathbb{R}^3 \rightarrow \mathbb{R}^3$ is piecewise affine such that*

$$e(\nabla v) \in U^{lc} \text{ a.e. in } \Omega.$$

Then there exists a Lipschitz map $u : \Omega \rightarrow \mathbb{R}^3$ such that

$$\begin{aligned} e(\nabla u) &\in U \text{ a.e. in } \Omega, \\ u &= v \text{ on } \partial\Omega. \end{aligned}$$

We remark that the Lipschitz constant of the map u strongly depends on the boundary data v . In fact, central factors playing a role, are the skew-symmetric part of

∇v as well as the order of lamination of $e(\nabla v)$.

In order to deal with *non-open* sets, we reduce the situation to the previously described case of open sets by working with the notion of “in-approximations”. Morally speaking, an in-approximation is a collection of bounded, open sets that can be reached by an application of Proposition 21 and which approximate the actual (non-open) set increasingly well. Thus, a countable number of iteration steps allows to deduce the desired existence result for the non-open situation.

We follow the notation of Müller and Šverák [MŠ99].

Definition 6. *Let $K \subset V$. A sequence $\{U_i\}_{i \in \mathbb{N}}$ of relatively open sets $U_i \subset V$ is an in-approximation of K in V if it satisfies*

1. *each U_i is uniformly bounded,*
2. *$U_i \subset U_{i+1}^{lc}$,*
3. *$U_i \rightarrow K$, i.e. if $F_i \in U_i$ converges to F this implies $F \in K$.*

In contrast to the geometrically nonlinear setting, the in-approximation will be applied to the strain (and not to the gradient), hence an additional tool for deducing compactness is necessary. This is provided by Korn’s inequality. Using the notion of an in-approximation, we prove the following proposition:

Proposition 22. *Let V be as above, $K \subset V$ and let $\{U_i\}_{i \in \mathbb{N}}$ be an in-approximation of K . Assume that $v : \Omega \subset \mathbb{R}^3 \rightarrow \mathbb{R}^3$ is piecewise affine and satisfies*

$$e(\nabla v) \in U_1 \text{ in } \Omega.$$

Then there exists $u : \Omega \rightarrow \mathbb{R}^3$, $u \in C^{0,\alpha}$ for all $\alpha \in [0, 1)$, such that

$$\begin{aligned} e(\nabla u) &\in K \text{ a.e. in } \Omega, \\ u &= v \text{ on } \partial\Omega. \end{aligned}$$

The unboundedness of the sets we are dealing with is reflected in weaker regularity properties of solutions of the differential inclusion (5.2.1): Instead of Lipschitz solutions as in the case of bounded gradient inclusions our ansatz only yields $C^{0,\alpha}$ solutions for any $\alpha \in [0, 1)$. This regularity property is derived via the boundedness of the inclusion in the set of symmetric matrices in combination with Korn’s inequality.

The loss of regularity is – in a weaker form – already contained in the first proposition. The strong dependence of the Lipschitz constant on the skew-symmetric part of ∇u , makes it difficult to carry out a countable iteration of Proposition 21 without losing the Lipschitz property.

Finally, Proposition 22 enables us to deal with the six-well problem and to conclude non-rigidity for the cubic-to-orthorhombic phase transition.

Corollary 2. *Let $e_1, \dots, e_6 \in \mathbb{R}_{sym}^{3 \times 3}$, $\text{tr}(e_i) = 0$, be such that $\dim(\text{intconv}(e_1, \dots, e_6)) = 5$ and such that there exist $a_{ij} \in \mathbb{R}^3 \setminus \{0\}$, $n_{ij} \in \mathbb{S}^2$ with*

$$e_i - e_j = \frac{1}{2}(a_{ij} \otimes n_{ij} + n_{ij} \otimes a_{ij}) \text{ for } i \neq j.$$

Then for any Lipschitz domain Ω and any $M \in \mathbb{R}^{3 \times 3}$ such that $\frac{1}{2}(M + M^t) \in \text{intconv}(e_1, \dots, e_6)$ there exists a function $u : \mathbb{R}^3 \rightarrow \mathbb{R}^3$, $u \in C^{0,\alpha}$ for all $\alpha \in [0, 1)$, satisfying

$$\begin{aligned} \nabla u &= M \text{ on } \mathbb{R}^3 \setminus \bar{\Omega}, \\ \frac{1}{2}(\nabla + \nabla^t)u &\in \{e_1, \dots, e_6\} \text{ a.e. in } \Omega. \end{aligned}$$

In particular, this result applies to the six-well problem and provides a very large set of highly irregular solutions to the inclusion problem associated with the cubic-to-orthorhombic phase transition.

The Case of the Rank-One Convex Hull

In the final part of Section 5.6 we deal with piecewise affine boundary conditions originating from the rank-one-convex hull of K , $v \in K^{rc}$. Although these boundary conditions include the previously discussed ones and it would have been possible to incorporate the first case into this one, we choose to present them separately as this final case causes additional technical difficulties.

Again, our strategy of proof leads to a loss in regularity. We only prove the results of Proposition 21 and 22 with the reduced $C^{0,\alpha}$ properties. The case involving rank-one convex hulls might, for example, be of interest for the cubic-to-monoclinic phase transition, c.f. [CS12].

The remainder of the chapter is organized as follows: Section 5.3 recalls the notions of lamination and rank-one convexity. Section 5.4 contains all auxiliary constructions, including the linearized Conti construction as well as various iterations of it. After this we reproduce the oscillation control lemma of Müller and Šverák [MŠ99], which forms the core of the convex integration procedure. Finally, in Section 5.6 we present the proofs of the results described above.

5.3 Preliminaries

Lamination Convexity

A crucial notion for the further discussion is (symmetrized) lamination convexity. Therefore, we briefly recall this notion, c.f. [Dac07], [MŠ99], [Kir07]. As we work in the framework of the linear theory of elasticity, we consider all notions adapted

to symmetric matrices (e.g. *symmetrized* rank-one-connections instead of rank-one-connections).

Definition 7. A set $U \subset \mathbb{R}_{sym}^{n \times n}$ is (symmetrized) lamination convex iff for any pair of (symmetrized) rank-one connected elements $a, b \in U$ the whole interval $[a, b]$ is contained in U . We denote the lamination convex hull of a set U by U^{lc} . It is characterized as the smallest lamination convex set containing U .

In the sequel we will make use of the following properties of the lamination convex hull:

- the lamination convex hull can be characterized as $U^{lc} = \bigcup_{j=0}^{\infty} \mathcal{L}_j(U)$, with

$$\begin{aligned} \mathcal{L}_0(U) &= U, \\ \mathcal{L}_j(U) &= \{c \in \mathbb{R}_{sym}^{n \times n}; c = \lambda a + (1 - \lambda)b, \lambda \in [0, 1], a, b \in \mathcal{L}_{j-1}(U), \\ &\quad \text{rank}(a - b) \leq 1\}. \end{aligned}$$

- If U is open, the same holds for $\mathcal{L}_j(U)$ for any $j \in \mathbb{N}$.
- If $n \in \mathbb{N}$ is minimal with $c \in \mathcal{L}_n(U)$ we denote it as the *order of lamination* (of c).

Rank-One Convexity

Since our strategy of proof displays strong enough robustness in order to apply it to the case of boundary data whose gradient originates from rank-one convex hulls, we recall the central aspects of this notion of convexity, c.f. [MŠ99]. We only deal with the case of symmetrized rank-one convex hulls. As above we make use of the notation $V = \{M \in \mathbb{R}_{sym}^{3 \times 3}, \text{tr}(M) = 0\}$.

Definition 8. • Let K be a compact subset of $\mathbb{R}_{sym}^{3 \times 3}$ (or of V). $X \in K^{rc}$ (or $X \in K_V^{rc}$) iff for any $f : \mathbb{R}_{sym}^{3 \times 3} \rightarrow \mathbb{R}$, which is symmetrized rank-one convex (on V), we have $f(X) \leq \sup_K f$.

- Let O be a bounded, (relatively) open subset of $\mathbb{R}_{sym}^{3 \times 3}$ (or of V). $X \in O^{rc}$ ($X \in O_V^{rc}$) iff there exists $K \subset O$, compact, such that $X \in K^{rc}$ ($X \in K_V^{rc}$).
- A probability measure μ supported on a compact set $K \subset \mathbb{R}_{sym}^{3 \times 3}$ is a laminate iff $\langle \mu, f \rangle \geq f(\bar{\mu})$ for any symmetrized rank-one convex function $f : \mathbb{R}_{sym}^{3 \times 3} \rightarrow \mathbb{R}$, where $\bar{\mu} = \int_{\mathbb{R}_{sym}^{3 \times 3}} \text{id}(Y) d\mu(Y)$. We denote the set of all such probability measures by $\mathcal{M}^{rc}(K)$.
- Let $O \subset \mathbb{R}_{sym}^{3 \times 3}$ ($O \subset V$) be (relatively) open. Then we define the collection of finite-order laminates as

$$\mathcal{L}(O) := \bigcup_{j=0}^{\infty} L_j(O),$$

where the $L_j(O)$ are defined inductively as sets of laminates of order j :

$$L_0(O) := \{\nu = \delta_A, A \in O\},$$

$$L_j(O) := \left\{ \nu = \sum_{k=1}^{j-2} \lambda_k \delta_{A_k} + \lambda_{j-1} s \delta_{B_0} + \lambda_{j-1} (1-s) \delta_{B_1}, \right.$$

such that there exists a probability measure $\nu' \in L_{j-1}(O)$ with

$$\nu' = \sum_{k=1}^{j-1} \lambda_k \delta_{A_k}, \quad A_{j-1} = sB_0 + (1-s)B_1, \quad s \in (0, 1),$$

and B_0, B_1 are symmetrized rank-one connected}.

Just as in the non-symmetrized situation, we have the following facts (c.f. [MŠ99], p.400):

- Let $K \subset V$, then $K_V^{rc} = \{\bar{\nu}; \nu \in \mathcal{M}^{rc}(K)\}$.
- Let $K \subset V$ be compact, $\nu \in \mathcal{M}^{rc}(K)$. Let $O \subset V$ be a (relatively) open set containing K_V^{rc} . Then there exists a sequence of finite laminates $\nu_j \in \mathcal{L}(O)$ such that

$$\begin{aligned} \nu_j &\xrightarrow{*} \nu \text{ in measure,} \\ \bar{\nu}_j &= \bar{\nu}. \end{aligned}$$

- For a (relatively) open set O the rank-one convex hull, O^{rc} (O_V^{rc}), remains (relatively) open.

5.4 Constructions

Conti's Construction: 2D and 3D

In this subsection we present “linearized” versions of a construction of Conti [Con08]. Instead of satisfying the determinant constraint appearing in the nonlinear setting, our construction with zero boundary data satisfies a zero trace condition. As in the original construction, we prove the statement in two steps: We first give a two-dimensional construction and then extend it to three dimensions.

In the two-dimensional setting we have:

Lemma 9. *Let $\lambda \in (0, 1)$, $\delta > 0$ and define*

$$M_0 = \begin{pmatrix} 0 & 0 \\ 1-\lambda & 0 \end{pmatrix}, \quad M_1 = \begin{pmatrix} 0 & 0 \\ -\lambda & 0 \end{pmatrix}.$$

Then there exists a piecewise affine Lipschitz map $u : \mathbb{R}^2 \rightarrow \mathbb{R}^2$ and domains $\Omega = \Omega_0 \cup \Omega_1$, Ω_1, Ω_0 (up to null sets) disjoint (each consisting of a union of triangles), such that

- ∇u attains at most five different values in Ω ,
- we have

$$\begin{aligned} \nabla \cdot u &= 0 \text{ in } \Omega, \\ u &= 0 \text{ in } \mathbb{R}^2 \setminus \bar{\Omega}, \end{aligned}$$

- it holds

$$\begin{aligned} |M_0 - \nabla u| &\leq \delta \text{ in } \Omega_0, \\ |M_1 - \nabla u| &\leq \delta \text{ in } \Omega_1. \end{aligned}$$

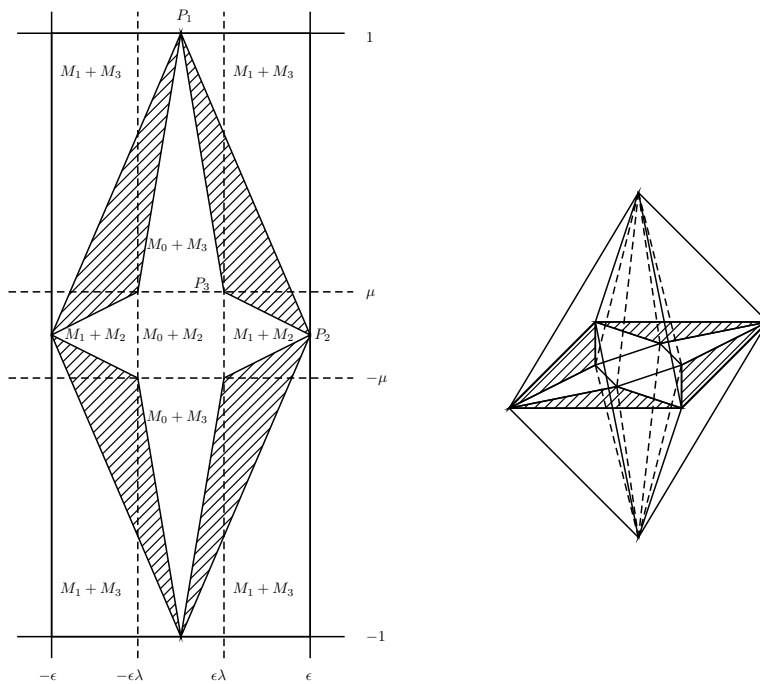


Figure 5.1: Conti's construction in 2D and 3D. The picture on the left describes the gradient distribution in the two-dimensional construction and depicts the triangles (dashed) where the construction is interpolated. The final domain Ω is given by the diamond. The picture on the right illustrates the extension of the construction to higher dimensions.

Proof. In analogy to Conti's construction in the nonlinear case [Con08], we construct the desired function in the diamond depicted in the left part of Figure 5.1. We first

focus on the construction in the first quadrant. The gradients of the functions

$$\begin{aligned} v^{M_0}(x) &:= \begin{pmatrix} 0 \\ (1-\lambda)x_1 \end{pmatrix}, & v^{M_1}(x) &:= \begin{pmatrix} 0 \\ -\lambda x_1 + \lambda\epsilon \end{pmatrix}, \\ v^{M_2}(x) &:= \begin{pmatrix} -q(1-\mu)x_2 \\ 0 \end{pmatrix}, & v^{M_3}(x) &:= \begin{pmatrix} q\mu x_2 - q\mu \\ 0 \end{pmatrix}, \end{aligned}$$

are given by

$$\begin{aligned} M_0 &= \begin{pmatrix} 0 & 0 \\ 1-\lambda & 0 \end{pmatrix}, & M_1 &= \begin{pmatrix} 0 & 0 \\ -\lambda & 0 \end{pmatrix}, \\ M_2 &= \begin{pmatrix} 0 & -q(1-\mu) \\ 0 & 0 \end{pmatrix}, & M_3 &= \begin{pmatrix} 0 & q\mu \\ 0 & 0 \end{pmatrix}. \end{aligned}$$

Due to the rank-one connections between M_0 , M_1 and M_2 , M_3 , respectively, it is possible to define a piecewise affine, continuous function \tilde{u} with the gradient distribution indicated in Figure 5.1:

$$\tilde{u}(x) = \begin{cases} v^{M_0}(x) + v^{M_2}(x) & \text{in } [-\epsilon\lambda, \epsilon\lambda] \times [-\mu, \mu], \\ v^{M_0}(x) + v^{M_3}(x) & \text{in } [-\epsilon\lambda, \epsilon\lambda] \times [\mu, 1], \\ v^{M_1}(x) + v^{M_2}(x) & \text{in } [\epsilon\lambda, \epsilon] \times [-\mu, \mu], \\ v^{M_1}(x) + v^{M_3}(x) & \text{in } [\epsilon\lambda, \epsilon] \times [\mu, 1]. \end{cases}$$

Furthermore, by the choice of the functions v^{M_i} , we obtain $\tilde{u}(P_2) = \tilde{u}(\epsilon, 0) = 0 = \tilde{u}(0, 1) = \tilde{u}(P_1)$. In order to obtain the desired conditions on the boundary of the diamond, we interpolate the values of \tilde{u} at P_1, P_2, P_3 linearly. This yields a new piecewise affine, continuous function u . By construction we have $u(P_1) = 0 = u(P_2)$, thus, u vanishes on the whole line segment connecting the points P_1 and P_2 . Moreover, by choosing $q = \frac{\lambda(1-\lambda)}{\mu(1-\mu)}\epsilon^2$, it is ensured that the resulting (interpolated) vector field remains divergence free (this can be seen by an application of Gauß's theorem or by the explicit computation of the gradient in the interpolation region). Thus, in the interpolated region the gradient of u can be computed to yield $\nabla u = p \begin{pmatrix} -\epsilon & -\epsilon^2 \\ 1 & \epsilon \end{pmatrix}$ with $p = -\lambda \frac{1}{1-\frac{\mu}{1-\lambda}} = -\lambda + O(\frac{\mu}{1-\lambda})$. On the remaining part of the first quadrant of the diamond, i.e. on the polygon defined by the points $P_1, (0, 0), P_2, P_3$, the gradient distribution of u coincides with that of \tilde{u} . Now the claim on the closeness of the gradients to the matrices M_0, M_1 follows by choosing

- $\mu = \epsilon$,
- $\epsilon > 0$ sufficiently small in dependence of λ and δ .

Carrying out similar considerations in the fourth quadrant, we obtain that the gradient in the corresponding interpolation region is given by $p \begin{pmatrix} \epsilon & -\epsilon^2 \\ 1 & -\epsilon \end{pmatrix}$. Finally, using the point symmetry of the overall construction, $u(x) = -u(-x)$, we obtain the desired construction involving only five gradients. \square

The two-dimensional Conti construction can be extended to an arbitrary dimension by inductively adding new points in each direction orthogonal to the already present $((n-1)$ -dimensional) building block. On these, the extended function is prescribed so as to satisfy the correct boundary conditions. The final higher-dimensional construction is obtained by interpolating between the “new points” and the lower dimensional construction (c.f. Figure 5.1, right part).

Lemma 10. *Let $\lambda \in (0, 1)$ and consider*

$$M_0 = \begin{pmatrix} 0 & 0 & 0 \\ 1 - \lambda & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad M_1 = \begin{pmatrix} 0 & 0 & 0 \\ -\lambda & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Then for any $\delta > 0$ there exists $\Omega \subset \mathbb{R}^3$, $\Omega = \Omega_0 \cup \Omega_1$ (each consisting of a finite, non-empty union of tetrahedra), and there exists a piecewise affine, Lipschitz map $u : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ such that

- ∇u takes on at most 10 different values in Ω ,
- we have

$$\begin{aligned} \nabla \cdot u &= 0 \text{ in } \Omega, \\ u &= 0 \text{ on } \mathbb{R}^2 \setminus \bar{\Omega}, \end{aligned}$$

- it holds

$$\begin{aligned} |M_0 - \nabla u| &\leq \delta \text{ on } \Omega_0, \\ |M_1 - \nabla u| &\leq \delta \text{ on } \Omega_1. \end{aligned}$$

Proof. We prove this lemma by applying the previous two-dimensional construction and an additional interpolation. In fact, considering the three-dimensional diamond given by the convex hull of the points

$$P_1 = (0, 1, 0), P_2 = (\epsilon, 0, 0), -P_1, -P_2, (0, 0, 1), (0, 0, -1),$$

we define $u(x) = \begin{pmatrix} u_1(x) \\ u_2(x) \\ 0 \end{pmatrix}$ by the previously constructed two dimensional function in the $\{x_3 = 0\}$ -plane. We extend it to the three-dimensional tetrahedron by setting $u(\pm e_3) = 0$ and interpolating in the resulting three-dimensional tetrahedra. As a consequence, we obtain at most 10 different gradients. Since $u_3(x) = 0$ on all of the vertices on which u is interpolated, we infer $u_3(x) = 0$ by linearity. Thus, the gradient of u reads

$$\nabla u = \begin{pmatrix} \nabla(u_1, u_2) & b \\ 0 & 0 \end{pmatrix}.$$

Combined with the divergence freeness of the two-dimensional matrix $\nabla(u_1, u_2)$, this demonstrates that the divergence freeness is preserved under the described interpolation procedure. \square

In order to control the volume distribution of the gradients/ symmetrized gradients appearing in Conti's construction, we use the following Lemma, which is again an adaptation of the nonlinear situation treated by Conti [Con08].

Lemma 11. *Let $\lambda \in (0, 1)$ and consider*

$$M_0 = \begin{pmatrix} 0 & 0 & 0 \\ 1 - \lambda & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad M_1 = \begin{pmatrix} 0 & 0 & 0 \\ -\lambda & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

For any $\delta > 0$ there exist domains $\Omega, \Omega_0, \Omega_1 \subset \mathbb{R}^3$, $\Omega = \Omega_0 \cup \Omega_1$ (each consisting of a finite union of tetrahedra and rectangular boxes), and a piecewise affine Lipschitz map $u : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ such that

- ∇u takes on at most 20 different values,
- we have

$$\begin{aligned} \nabla \cdot u &= 0 \text{ in } \Omega, \\ u &= 0 \text{ on } \mathbb{R}^3 \setminus \bar{\Omega}, \end{aligned}$$

- it holds

$$\begin{aligned} |M_0 - \nabla u| &\leq \delta \text{ on } \Omega_0, \\ |M_1 - \nabla u| &\leq \delta \text{ on } \Omega_1, \end{aligned}$$

- the volume fractions satisfy

$$|\{x \in \Omega; \nabla u \notin \{M_0, M_1\}\}| \leq \delta |\Omega|.$$

Proof. We follow the ideas of Conti. Defining $u^{(1)}$ as the function from Lemma 10, we set

$$u^{(k)}(x) := \begin{cases} u^{(k-1)}(x - Le_k), & x_k > L, \\ u^{(k-1)}(x - x_k), & |x_k| \leq L, \\ u^{(k-1)}(x + Le_k), & x_k < -L, \end{cases}$$

for $k \in \{2, 3\}$ and $L > 0$ sufficiently large, to be chosen later. By definition, this is a Lipschitz function. Its gradient remains unchanged for $|x_k| \geq L$, while the structure of M_0, M_1 implies $\nabla u \in \{M_0, M_1\}$ for $|x_k| \leq L$. Finally, choosing $L = L(\delta)$ sufficiently large, also yields the claim on the volume fractions. \square

Remark 21. Such a precise volume control as provided by the previous lemma is actually only needed when dealing with the case of rank-one convex hulls. Since it does not impose additional technical difficulties, it is included already in the simpler context of lamination convex hulls.

Application of Conti's Construction to General Rank-One Connected Matrices

In this section we illustrate that Conti's construction can be generalized to satisfy arbitrary boundary conditions and to take on prescribed gradient values (up to a previously determined error) in certain tetrahedra. With this construction, we obtain a function which satisfies the correct boundary condition and whose interior gradient configuration is modified along a rank-one segment.

Lemma 12 (Deformation of Conti's Construction). *Let $\delta > 0$ and assume that $M \in \mathbb{R}^{3 \times 3}$, $\text{tr}(M) = 0$, such that there exist $a \in \mathbb{R}^3 \setminus \{0\}$, $n \in \mathbb{S}^2$, $M_0, M_1 \in \mathbb{R}^{3 \times 3}$, $\lambda \in (0, 1)$ with*

$$\begin{aligned} M &= \lambda M_0 + (1 - \lambda)M_1, \\ M_1 - M_0 &= a \otimes n, \quad a \cdot n = 0. \end{aligned}$$

Then there exist sets $\Omega, \Omega_0, \Omega_1 \subset \mathbb{R}^3$, $\Omega = \Omega_0 \cup \Omega_1$; Ω_0, Ω_1 each being a union of finitely many tetrahedra, and there exists a piecewise affine Lipschitz function $u : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ satisfying:

- *the gradient of u attains at most 20 different values; it is constant on the tetrahedra which are the components of Ω_0 and Ω_1 ,*
- $\nabla u = M$ in $\mathbb{R}^3 \setminus \bar{\Omega}$,
- $\nabla \cdot u = 0$,
- $|\nabla u - M_0| \leq \delta$ on Ω_0 , $|\nabla u - M_1| \leq \delta$ on Ω_1 ,
- $|\{x \in \Omega; \nabla u \notin \{M_0, M_1\}\}| \leq \delta|\Omega|$.

Proof. By a translation in matrix-space, a rotation in x -space and a rescaling in u -space we may assume

$$M = 0, \quad n = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad a = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}.$$

Hence, we obtain

$$M_0 = \begin{pmatrix} 0 & 0 & 0 \\ 1 - \lambda & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad M_1 = \begin{pmatrix} 0 & 0 & 0 \\ -\lambda & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Now the claim follows from an application of Conti's construction, Lemma 11. \square

Rank-One-Connections from Symmetrized Rank-One-Connections in \mathbb{R}^3

In constructing the in-approximation, it will be necessary to move the involved strains closer and closer to the strains of the approximated set K . In order to do so, we intend to apply the deformed Conti construction iteratively. As the first step consists of finding the "right" rank-one connected matrices (M_0 and M_1 in Lemma 12), the following gives a characterization of the property of being rank-one-connected.

Lemma 13. *Let $e_i \in \mathbb{R}_{sym}^{3 \times 3}$, $\text{tr}(e_i) = c$, $i \in \{0, 1\}$, $e_0 \neq e_1$. Then the following statements are equivalent:*

1. *There exist matrices M_0, M_1 and vectors $a \in \mathbb{R}^3 \setminus \{0\}, n \in \mathbb{S}^2$ such that*

$$\begin{aligned} \frac{1}{2}(M_i + M_i^t) &= e_i, \quad i \in \{0, 1\}, \\ M_0 - M_1 &= a \otimes n, \quad a \perp n. \end{aligned}$$

2. *There exist vectors $a \in \mathbb{R}^3 \setminus \{0\}, n \in \mathbb{S}^2$ such that*

$$e_1 - e_0 = \frac{1}{2}(a \otimes n + n \otimes a).$$

3. *It holds $\det(e_1 - e_0) = 0$.*

Proof. The statements $1 \Rightarrow 2 \Rightarrow 3$ and $2 \Rightarrow 1$ are clear. It remains to prove that the third statement implies the second. As $e_1 - e_0$ is symmetric, there exist orthonormal eigenvectors $v_1, v_2, v_3 \in \mathbb{S}^2$ with eigenvalues $\lambda_1, \lambda_2, \lambda_3 \in \mathbb{R}$ such that

$$e_1 - e_0 = \lambda_1 v_1 \otimes v_1 + \lambda_2 v_2 \otimes v_2 + \lambda_3 v_3 \otimes v_3.$$

As the determinant vanishes, we may assume that $\lambda_3 = 0$. Furthermore, the condition on the traces of the strains, e_i , implies $\text{tr}(e_1 - e_0) = 0$, leading to $\lambda_2 = -\lambda_1 =: -\lambda$. Hence,

$$\begin{aligned} e_1 - e_0 &= \lambda(v_1 \otimes v_1 - v_2 \otimes v_2) \\ &= \frac{\lambda}{2}((v_1 + v_2) \otimes (v_1 - v_2) + (v_1 - v_2) \otimes (v_1 + v_2)) \\ &= \frac{1}{2}(a \otimes n + n \otimes a), \end{aligned}$$

for $n := v_1 - v_2$, $a := \lambda(v_1 + v_2)$ (a reversal of the signs in a , n would also have been possible). \square

Remark 22. • In an arbitrary dimension, d , the first two statements remain equivalent. The third condition becomes a necessary but not sufficient condition.

- The choice $n = v_1 - v_2$, $a = \lambda(v_1 + v_2)$ implies a bound for the skew symmetric part $S = \frac{1}{2}(a \otimes n - n \otimes a)$ of $M_1 - M_0$: $|S| \leq 4|\lambda|$.

With the previous lemma we have obtained a necessary and sufficient condition for (symmetric) rank-one-connectedness. This will be applied to the strains contained in the wells. We will move an arbitrary strain in the interior of the lamination convex hull of the wells closer and closer to the extreme points, i.e. the wells.

The procedure we apply is iterative in the sense that we first show that a given strain in $\mathcal{L}_i(U)$ can be moved towards $\mathcal{L}_{i-1}(U)$. This is the content of Lemma 14.

Lemma 14. *Let $M \in \mathbb{R}^{3 \times 3}$, $tr(M) = 0$, $e_0, e_1 \in \mathbb{R}_{sym}^{3 \times 3}$, $tr(e_i) = 0$ and assume that the matrices $e_0 \neq e_1$ are symmetrized rank-one-connected such that for $\tilde{e} := e(M)$ there exists $\lambda \in (0, 1)$ with*

$$\tilde{e} = \lambda e_0 + (1 - \lambda)e_1.$$

Then there exist $M_0, M_1 \in \mathbb{R}^{3 \times 3}$, $a \in \mathbb{R}^3 \setminus \{0\}$, $n \in \mathbb{S}^2$ such that

$$\begin{aligned} e(M_0) &= e_0, \\ e(M_1) &= e_1, \\ M_1 - M_0 &= a \otimes n, \quad a \cdot n = 0, \\ M &= \lambda M_0 + (1 - \lambda)M_1. \end{aligned}$$

Proof. By an application of Lemma 13 we obtain a skew symmetric matrix \bar{S} and vectors $a \in \mathbb{R}^3 \setminus \{0\}$, $n \in \mathbb{S}^2$ such that

$$e_1 - e_0 + \bar{S} = a \otimes n.$$

Setting $S(M) := \frac{1}{2}(M - M^t)$, we have

$$\begin{aligned} M &= \lambda(e_0 + S(M)) + (1 - \lambda)(e_1 + S(M)) \\ &= \lambda(e_0 + S(M) + (1 - \lambda)\tilde{S}) + (1 - \lambda)(e_1 + S(M) - \lambda\tilde{S}), \end{aligned}$$

for an arbitrary skew symmetric matrix \tilde{S} . Choosing $\tilde{S} := \bar{S}$ and setting

$$\begin{aligned} M_0 &:= e_0 + S(M) - (1 - \lambda)\bar{S}, \\ M_1 &:= e_1 + S(M) + \lambda\bar{S}, \end{aligned}$$

yields the desired rank-one-connected matrices. □

5.5 Controlled Convergence Lemma

The key to the overall construction is provided by the “oscillation control lemma” of Müller and Šverák [MŠ99]. It states that a very strong L^∞ control allows to improve weak $W^{1,p}$, $p > 1$, convergence to strong $W^{1,1}$ convergence. The central idea is a “separation of scales”: While the gradient may vary on scales of order one, the L^∞ bound implies that these oscillations take place on an extremely small spatial scale. Simultaneously, a convolution bound ensures that this scale is not arbitrarily small, which avoids the danger of creating only *weak* – and not *strong* – convergence.

Lemma 15 (Müller-Šverák). *Let $\Omega \subset \subset \mathbb{R}^n$ be a bounded set, $\rho \in C_0^\infty(\Omega)$, $\rho_\epsilon(x) := \frac{1}{\epsilon^n} \rho(\frac{x}{\epsilon})$, $\int_\Omega \rho dx = 1$, $\rho \geq 0$. Suppose that v is a piecewise affine function on Ω . Assume that $u_j : \Omega \rightarrow \mathbb{R}^n$ is a sequence satisfying*

$$\begin{aligned} \|u_j\|_{W^{1,p}(\Omega)} &\leq C < \infty \text{ for some } p > 1, \\ u_j &= v \text{ on } \partial\Omega, \\ \|\nabla u_j * \rho_{\epsilon_j} - \nabla u_j\|_{L^1(\Omega)} &\leq 2^{-j}, \\ \delta_{j+1} &= \epsilon_j \delta_j, \quad \delta_0 \leq 1, \quad \epsilon_j \leq 2^{-(j+1)}, \\ \|u_{j+1} - u_j\|_{L^\infty(\Omega)} &\leq \delta_{j+1}, \quad u_0 = v, \\ \|u_{j+2} - u_{j+1}\|_{L^\infty(\Omega)} &\leq \frac{\|u_{j+1} - u_j\|_{L^\infty(\Omega)}}{2}. \end{aligned}$$

Then

$$u_j \rightarrow u_\infty \text{ in } L^\infty(\Omega) \cap W^{1,1}(\Omega) \text{ as } j \rightarrow \infty.$$

Proof. We follow the proof of Müller & Šverák [MŠ99]. Denoting $u_{j+1} - u_j =: \phi_j$ and considering the geometric bounds on δ_j we have the estimate

$$\|u_j - u_{j'}\|_{L^\infty} \leq \sum_{\min\{j,j'\}}^{\infty} \|\phi_j\|_{L^\infty} \leq 2 \|\phi_{\min\{j,j'\}}\|_{L^\infty}.$$

Thus, there exists u_∞ such that $u_j \rightarrow u_\infty$ in L^∞ . Due to the boundedness of the $W^{1,p}$ norm and the L^∞ convergence, we may further assume $u_j \rightharpoonup u_\infty$ in $W^{1,p}$. We prove strong convergence in $W^{1,1}$:

$$\begin{aligned} \|\nabla(u_j - u_\infty)\|_{L^1(\Omega)} &\leq \|\nabla u_j - \nabla u_j * \rho_{\epsilon_j}\|_{L^1(\Omega)} + \|\nabla u_\infty * \rho_{\epsilon_j} - \nabla u_\infty\|_{L^1(\Omega)} \\ &\quad + \|\nabla u_j * \rho_{\epsilon_j} - \nabla u_\infty * \rho_{\epsilon_j}\|_{L^1(\Omega)}. \end{aligned}$$

Here the first term converges to zero by the assumptions, while the second one converges by properties of convolution. For the third term we make use of the

strong L^∞ control. Denoting $\Omega_j := \{x : \text{dist}(x, \partial\Omega) > 2\epsilon_j\}$, we have

$$\begin{aligned} \|\nabla u_j * \rho_{\epsilon_j} - \nabla u_\infty * \rho_{\epsilon_j}\|_{L^1(\Omega)} &= \|\nabla u_j * \rho_{\epsilon_j} - \nabla u_\infty * \rho_{\epsilon_j}\|_{L^1(\Omega_j)} \\ &\quad + \|\nabla u_j * \rho_{\epsilon_j} - \nabla u_\infty * \rho_{\epsilon_j}\|_{L^1(\Omega \setminus \Omega_j)}. \end{aligned}$$

The second term on the right hand side can be bounded by means of Young's inequality combined with the smallness of $|\Omega \setminus \Omega_j|$ and the uniform $W^{1,p}$ assumption on the u_j . For the first term we apply the following estimate:

$$\begin{aligned} \|\nabla u_j * \rho_{\epsilon_j} - \nabla u_\infty * \rho_{\epsilon_j}\|_{L^1(\Omega_j)} &= \|(u_j - u_\infty) * \nabla \rho_{\epsilon_j}\|_{L^1(\Omega_j)} \\ &\leq \frac{1}{\epsilon_j} \|u_j - u_\infty\|_{L^\infty(\Omega)}. \end{aligned}$$

Since by assumption

$$\|u_j - u_\infty\|_{L^\infty(\Omega)} \leq 2 \|u_j - u_{j+1}\|_{L^\infty(\Omega)} \leq 2\epsilon_j \delta_j,$$

also the last term can be made arbitrarily small for sufficiently large j . \square

By invoking Conti's construction in successively building up a Müller-Šverák sequence, i.e. a sequence satisfying the conditions of the controlled convergence lemma, it will be relatively easy to obtain improved volume fractions on which the strains are closer and closer to the desired sets. However, the necessary difference in the displacements will not automatically be small. As a consequence the following construction will repeatedly play an essential role, allowing to change the L^∞ norm of a function and preserving the gradient distribution at the same time.

Remark 23 (Vitali-Construction). Let $f : \Omega \rightarrow \mathbb{R}^m$, $f \in W_0^{1,\infty}(\Omega)$. Partitioning Ω into rescaled copies of Ω of side length ϵ_i , $\Omega = \bigcup_i^\infty \Omega_i := \bigcup_i^\infty (x_i + \epsilon_i \Omega)$, and setting $u(x) := \epsilon_i f(\frac{x-x_i}{\epsilon_i})$, yields a function which has the same gradient distribution in Ω as f and which satisfies the L^∞ estimate

$$\|u\|_{L^\infty(\Omega_i)} \leq \epsilon_i \|f\|_{L^\infty(\Omega_i)}.$$

This construction makes it possible to preserve a gradient distribution while improving the L^∞ control.

5.6 Proofs of Propositions 21 & 22, Corollary 2

Finally, we combine the previous considerations and construct a Müller-Šverák sequence with the in-approximation properties.

Proof of Proposition 21

Proof of Proposition 21. Let $\Omega \subset\subset \mathbb{R}^3$ be a bounded set, $U \subset \mathbb{R}_{sym}^{3 \times 3}$ open, trace-free, $v : \Omega \rightarrow \mathbb{R}^3$ piecewise affine such that

$$e(\nabla v) \in U^{lc}.$$

Without loss of generality, we may assume that v is affine (else we restrict to the affine parts), $v = Mx$.

We construct a solution of the inclusion problem via iteration. Setting $u_1 := Mx$, we modify this function by applications of Conti's construction.

By Whitney's decomposition theorem for any $\epsilon > 0$ we obtain a disjoint covering of $\Omega := \bigcup_{j=1}^{\infty} (\epsilon_j \Omega_\epsilon + b_j) = \bigcup_{j=1}^{\infty} \Omega_j$ by translated and rescaled versions of the domains, Ω_ϵ , used in Lemma 12.

Since $e(M) \in U^{lc}$ there exists $n = n(M) < \infty$ such that $e(M) \in \mathcal{L}_n(U)$. As a consequence, it is possible to find $e_0, e_1 \in \mathcal{L}_{n-1}(U)$, symmetrized rank-one-connected, such that

$$e(M) = \lambda e_0 + (1 - \lambda) e_1.$$

For each $k \in \mathbb{N}$, we apply Lemma 14 combined with Lemma 12 on Ω_k . This yields a Lipschitz function $u_2^k : \Omega_k \rightarrow \mathbb{R}^3$ as well as a partition of Ω_k into Ω_0^k and Ω_1^k , each being a finite union of tetrahedra satisfying

$$u_2^k = Mx + \phi_1^k \text{ on } \Omega_k,$$

with $\phi_1^k \in W_0^{1,\infty}(\Omega_k)$. Combining the functions u_2^k , $u_2 = \sum_{k \in \mathbb{N}} u_2^k$, we have

$$\begin{aligned} \nabla u_2 &= M \text{ on } \mathbb{R}^3 \setminus \bar{\Omega}, \\ \nabla \cdot u_2 &= 0 \text{ on } \mathbb{R}^3, \\ u_2 &= Mx + \phi_1 \text{ on } \Omega, \end{aligned}$$

where $\phi_1 \in W_0^{1,\infty}$ is piecewise affine taking on at most 20 different values for its gradient. Moreover, $e(\nabla u_2)$ is close to $\mathcal{L}_{n-1}(U)$:

$$e(\nabla u_2) = e_j + e_{\delta_1}^j, \quad j \in \{0, 1\}$$

with $|e_{\delta_1}^j| \leq \delta$. Choosing $\epsilon = \epsilon(\delta, M, U)$ sufficiently small, we deduce $e(\nabla u_2) \in \mathcal{L}_{n-1}(U)$, as the openness of U implies the openness of $\mathcal{L}_{n-1}(U)$ (c.f. Section 5.3).

On the rescaled tetrahedra on which the gradient is constant, we iterate the construction described above. Since now $e(\nabla u_2) \in \mathcal{L}_{n-1}(U)$, we deduce that $n - 2$

further steps yield Lipschitz functions $\phi_{n-1} \in W_0^{1,\infty}(\Omega)$, $u_{n-1} : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ such that

$$\begin{aligned} \nabla u_{n-1} &= M \text{ on } \mathbb{R}^3 \setminus \bar{\Omega}, \\ u_{n-1} &= Mx + \phi_{n-1} \text{ on } \Omega, \\ e(\nabla u_{n-1}) &\in U \text{ in } \Omega. \end{aligned}$$

This implies the desired conclusion. \square

Remark 24. By an application of Vitali's theorem the construction described above shows that for any $\delta > 0$ it is possible to obtain an L^∞ bound of the form

$$\|u - v\|_{L^\infty} \leq \delta$$

for the solution u of the differential inclusion with boundary data v .

Proof of Proposition 22

Proof of Proposition 22. Without loss of generality, we may again assume that $u = Mx$ on $\partial\Omega$. We iterate the construction described in the previous proof. In fact, by the first two properties of in-approximations and an application of Proposition 21, it is possible to choose $u_i : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ such that

$$\begin{aligned} e(\nabla u_i) &\in U_i \text{ in } \Omega, \\ u_i &= u_{i-1} \text{ on } \partial\Omega, \\ \|u_i - u_{i-1}\|_{L^\infty(\Omega)} &\leq \delta_i, \end{aligned}$$

for arbitrary, given $\delta_i > 0$. In order to apply the Müller-Šverák Lemma which would allow to iterate Proposition 21 and still obtain a convergent subsequence, we have to deduce L^p bounds on the resulting gradients. Although Proposition 21 yields Lipschitz solutions, the Lipschitz constants are not uniform. On the contrary, they strongly depend on the order of lamination of the boundary data and on the skew-symmetric part of the boundary data. Hence, instead of deriving L^∞ bounds for the gradient, we refer to Korn's inequality, c.f. [KO88], [CDM12]: As for each $i \in \mathbb{N}$, $e(\nabla u_i) \in U^{lc}$ and U^{lc} is bounded, we infer via Korn's inequality that

$$\{\nabla u_i - M\}_i \text{ is bounded in } L^p(\mathbb{R}^3), \text{ for all } p \in (1, \infty).$$

As a result, for any $p \in (1, \infty)$ we can rely on uniform bounds for $\|u_i\|_{W^{1,p}(\Omega)}$. Furthermore, in each iteration step, $\epsilon_i > 0$ can be chosen such that

$$\|\nabla u_i * \rho_{\epsilon_i} - \nabla u_i\|_{L^1(\Omega)} \leq 2^{-i}.$$

Thus, the sequence u_i can be constructed satisfying the assumptions of the Müller-

Šverák Lemma, i.e.

$$\begin{aligned}
\|u_i\|_{W^{1,p}(\Omega)} &\leq C(p) < \infty, \quad p > 1, \\
u_i &= Mx \text{ on } \partial\Omega, \\
\|\nabla u_i * \rho_{\epsilon_i} - \nabla u_i\|_{L^1(\Omega)} &\leq 2^{-i}, \\
\delta_{i+1} &= \epsilon_i \delta_i, \quad \delta_0 \leq 1, \quad \epsilon_i \leq 2^{-(i+1)}, \\
\|u_{i+1} - u_i\|_{L^\infty(\Omega)} &\leq \delta_{i+1}, \quad \|u_{j+2} - u_{j+1}\|_{L^\infty(\Omega)} \leq \frac{\|u_{j+1} - u_j\|_{L^\infty(\Omega)}}{2}, \\
\int_{\Omega} \text{dist}(e(\nabla u_i), K) dx &\leq \frac{C}{2^{i-2}}.
\end{aligned}$$

Combining the statement of the Müller-Šverák Lemma and the third property of the in-approximation, this implies that for all $p \in (1, \infty)$ there exists $u \in W_{loc}^{1,p}(\mathbb{R}^3)$, such that (up to a subsequence)

$$\begin{aligned}
u_i &\rightarrow u \text{ in } W_{loc}^{1,1}(\mathbb{R}^3), \\
u &= Mx \text{ on } \partial\Omega, \\
e(\nabla u_i) &\rightarrow K \text{ in } L^1.
\end{aligned}$$

Hence, $e(\nabla u) \in K$, which proves the proposition. \square

Proof of Corollary 2

Proof of Corollary 2. By Proposition 22 it suffices to construct an appropriate in-approximation to the problem. In order to construct this, we remark that due to the (pairwise symmetrized) rank-one connectedness of the matrices the (symmetrized) rank-one-convex hull agrees with the convex hull of the strains:

$$\{e_1, \dots, e_6\}^{lc} = \{e_1, \dots, e_6\}^{co}.$$

Thus, an in-approximation of $\{e_1, \dots, e_6\}$ is provided by

$$\begin{aligned}
U_1 &:= \text{intconv}\{e_1, \dots, e_6\}, \\
U_k^j &:= \{x : \text{dist}(x, e_j) < \epsilon_k\} \cap \text{intconv}\{e_1, \dots, e_6\}, \\
U_k &:= \bigcup_{j=1}^6 U_k^j,
\end{aligned}$$

for $\epsilon_k > 0$ such that $\epsilon_k \rightarrow 0$ as $k \rightarrow \infty$. The first and third properties of an in-approximation are satisfied by definition. The second one follows from the symmetrized rank-one-connectedness of the strains, e_j . \square

The Case of Rank-One-Convex Hulls

Also the inclusion problem with boundary conditions originating from the rank-one-convex hull can be studied with the methods from the previous sections. The results of Chenchiah & Schlömerkemper [CS12] indicate that this might be necessary in order to deal with the cubic-to-monoclinic phase transition.

We formulate the central approximation lemma which corresponds to Lemma 4.1 in [MŠ99]. Instead of gradients, we have to consider symmetrized gradients.

Lemma 16. *Let $\epsilon > 0$ and let $O \subset V$ be relatively open, $F \in \mathbb{R}^{3 \times 3}$ such that $e(F) \in O_V^{rc}$. Then there exists a piecewise affine map $u : \Omega \subset \mathbb{R}^3 \rightarrow \mathbb{R}^3$ such that $e(\nabla u) \in O_V^{rc}$ a.e. in Ω and*

$$\begin{aligned} |\{e(\nabla u) \notin O\}| &\leq \epsilon |\Omega|, \\ u &= Fx \text{ on } \partial\Omega. \end{aligned} \tag{5.6.1}$$

Proof. As in the argument of Müller and Šverák [MŠ99], this statement is proven inductively. Let $F \in \mathbb{R}^{3 \times 3}$ with $e(F) \in O^{rc}$ be given. By definition of the rank-one convex hull there exists a compact set $K \subset V$ such that $e(F) \in K^{rc}$. Therefore, the characterization of the rank-one convex hull via laminates implies that there exists $\nu \in \mathcal{M}^{rc}(K)$ such that $F = \bar{\nu}$. By the approximation argument of Müller and Šverák there exists a sequence $\nu_j \in \mathcal{L}(O)$ such that $\nu_j \xrightarrow{*} \nu$, $\bar{\nu}_j = e(F)$. In order to prove the lemma, we distribute the masses according to the measure ν . For the general case we argue by induction: If $\nu = \lambda_1 \delta_{e_1} + \lambda_2 \delta_{e_2}$ Lemma 11 together with a covering argument yields the existence of a function $u : \Omega \rightarrow \mathbb{R}^3$ such that

$$|\{ |e(\nabla u) - A_i| \leq \delta \}| - \lambda_i |\Omega| \leq \epsilon,$$

for any $\epsilon > 0$.

Let $\nu_n := \sum_{j=1}^{n-2} \lambda_j \delta_{A_j} + s \lambda_n \delta_{A_n^1} + (1-s) \lambda_n \delta_{A_n^2}$ be a laminate of finite order. Then the inductive hypothesis allows to assume that there exists a laminate $\nu_{n-1} = \sum_{j=1}^{n-1} \lambda_j \delta_{A_j}$ with the property that $A_{n-1} = s A_n^1 + (1-s) A_n^2$, A_n^1, A_n^2 being symmetrized rank-one connected. Furthermore, the inductive hypothesis yields

$$|\{ |e(\nabla u) - A_i| \leq \delta \}| - \lambda_i |\Omega| \leq \epsilon, \quad i \in \{1, \dots, n-1\}.$$

Let E_n be the set on which $|e(\nabla u) - A_{n-1}| \leq \delta$. On each of the components on which $e(\nabla u)$ is affine, we apply Lemma 9 with the strains $A_n^k - (e(\nabla u) - A_{n-1})$, $k \in \{1, 2\}$. This yields the desired approximation corresponding to ν_j . Since O^{rc} is open and due to the convergence of ν_j to ν , there exists $j \in \mathbb{N}$ such that (5.6.1) is satisfied. \square

Using this lemma, the arguments for Propositions 21, 22 with boundary data in

U^{rc} , K^{rc} , respectively, follow as in the previous proofs by an application of the $W^{1,p}$ bounds obtained by Korn's inequality.

Chapter 6

Rigidity of Piecewise Polygonal Configurations

6.1 Introduction

As pointed out in the previous chapter – morally speaking – convex integration techniques yield “physically unrealistic, wild” solutions of the differential inclusion (4.0.1). Complementary to this, results from the literature indicate that combining the n -well problem with a regularity constraint on the deformation or on the strain allows to recover rigidity, c.f. [DM95a], [Kir98]. We pursue this philosophy in the sequel in its most primitive form: We investigate the differential inclusion (4.0.1) under the assumption of dealing with piecewise polygonal phase distributions, i.e. the support of each phase only consists of a *finite* (but arbitrarily large) number of polygons. In this case we prove that locally the most complicated, compatible, exactly stress-free configurations are crossing twins.

Overview of the Previously Existing Results and Methods

As reviewed in the previous chapter, it is not unusual that non-rigidity results for a partial differential inclusion can be complemented by rigidity results under additional regularity requirements. In the sequel we recall some of the techniques which are used in the literature.

- **The Two-Well Problem.** As already described, the nonlinear two-well problem does not feature rigidity in general. However, it is possible to recover this property if additional BV conditions are imposed, c.f. [DM95b]. Dolzmann and Müller approach this rigidity property by “linearizing” the nonlinear problem: The BV conditions allow to extract information from the nonlinear compatibility equations in order to give an explicit description of the jump set of the strain gradient. Then the commutativity of the group $SO(2)$ can be exploited for a “linearization” procedure.

- **The Cubic-to-Tetragonal Phase Transition.** In the case of the three-dimensional cubic-to-tetragonal phase transition, the strategy of Dolzmann and Müller cannot be pursued any more, as, in contrast to the rotations of \mathbb{R}^2 , the group $SO(3)$ of rotations of \mathbb{R}^3 is no longer commutative. As a consequence, the “linearization” technique cannot be applied any more. Instead, Kirchheim [Kir98] uses a more combinatorial approach: Referring to the explicit structure of the normals involved in the phase transition, combined with (general) properties of BV functions, he tackles the problem.

For our problem neither of the strategies seems to be applicable: The approach of Dolzmann & Müller does not provide a suitable framework as the non-rigidity phenomena occur in the *linear* model in our situation. Thus, there is no immediate chance of reducing the model to a simpler differential inclusion with stronger rigidity properties. Furthermore, the ideas of Kirchheim strongly rely on the structure of the cubic-to-tetragonal phase transition and its relatively small number of rank-one connections.

However, instead of facing six different normals, each *uniquely* associated with a single jump, we are confronted with 21 different normals, allowing for *non-unique* jumps. As a result, we choose a different strategy in order to deal with the problem: Motivated by considerations concerning two-dimensional toy models and by having good compatibility conditions for two-dimensional homogeneous corners, we first investigate the homogeneous situation (which can be considered as the blow-up of the more general piecewise polygonal case). Then, combinatorial considerations allow to carry these local insights over to the global situation of piecewise polygonal configurations.

Bifurcations with Respect to the Different Parameters for δ

In studying the cubic-to-orthorhombic phase transition, it is interesting to understand the behaviour of patterns in their dependence on the parameter δ , c.f. Figure 6.1. As we will see in the sequel, this changes very discontinuously at certain discrete values. In fact, exceptional cases are given by $\delta \in \{0, \pm\frac{3}{2}, \pm 3\}$. In all the other cases – and in this sense we refer to these parameters as being “generic” – the behaviour of the emerging patterns is comparable: Here, possible configurations have at most the complexity of crossing twin structures. Moreover, in all these cases there are explicit examples of patterns consisting exactly of crossing twins.

If one compares these crossing twins, one realizes that there are (up to symmetries) essentially two different cases, c.f. Figures 6.4, 6.5, 6.6 in Section 6.6. In the first case (including e.g. configurations *K1* and *K3* in Figure 6.4) the situation collapses to the usual laminate construction for $\delta \rightarrow 0$. However, the situation is different in the second case (including e.g. configuration *K2* in Figure 6.4): There is no continuous transition from $\delta > 0$ to the laminate situation of $\delta = 0$. In this second situation the slopes of the inner twins converge against the slopes of the outer twins. Instead of combining two phases which both collapse to the same variant of

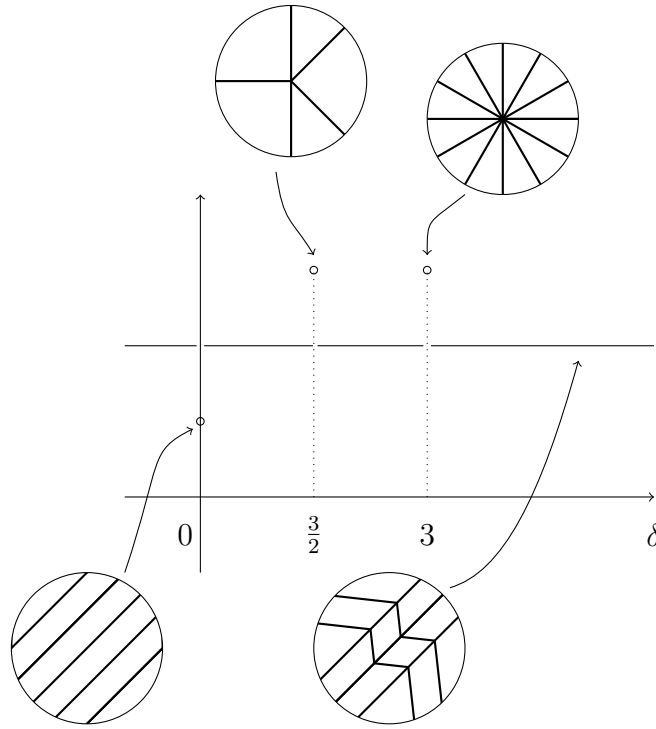


Figure 6.1: The generic behavior of possibly emerging patterns in dependence of the parameter δ .

martensite in the limit $\delta \rightarrow 0$, the individual inner twins “form new bands”.

Regarding the non-generic situations $\delta \in \{0, \pm\frac{3}{2}, \pm 3\}$, the simplest case consists of $\delta = 0$. As this (formally) corresponds to the cubic-to-tetragonal phase transition, the results of Dolzmann & Müller [DM95a] imply that the possible patterns are less complex than in the generic situation: Locally, at most laminates occur. The remaining cases $\delta \in \{\pm\frac{3}{2}, \pm 3\}$ display a much greater variety of different configurations. This is a result of various normals coinciding or falling into the same planes in these situations (c.f. Section 6.7 for a brief discussion).

6.2 The Main Results

Let us now describe the main results and the methods of our proof. We are interested in classifying the possibly emerging stress-free patterns for generic δ – i.e. $\delta \notin \{\pm\frac{3}{2}, \pm 3\}$. From the discussion of our model, c.f. Section 4.2, we know that:

- All of the strains determining the cubic-to-orthorhombic phase transition are pairwise (symmetrized) rank-one connected via two possible normals, i.e. for each $i \neq j$ there exist vectors $a_{ij} \in \mathbb{R}^3 \setminus \{0\}$, $n_{ij} \in \mathbb{S}^2$ with the property

$$e^{(i)} - e^{(j)} = \frac{1}{2}(a_{ij} \otimes n_{ij} + n_{ij} \otimes a_{ij}). \quad (6.2.1)$$

- Thus, possible non-constant configurations of these strains are, for example,

given by laminates, i.e. twin configurations jumping at the normals determined by (6.2.1).

- In contrast to other martensitic phase transitions such as the cubic-to-tetragonal transition, laminates do not constitute the only possible configurations. On the contrary, so-called crossing twin structures can form as well (c.f. Fig. 4.3).

The main result of this chapter states that, generically, twins and crossing twins are the only possible configurations; in particular, more complicated structures can be excluded. In fact, we prove the following statement:

Proposition 23. *Let $\delta \notin \{\pm\frac{3}{2}, \pm 3\}$. Assume that $\Omega \subset \mathbb{R}^3$ is a Lipschitz domain. Then any piecewise polygonal strain with*

$$e(\nabla u) \in \{e^{(1)}, \dots, e^{(6)}\} \text{ in } \Omega,$$

is locally either given by a laminate or a crossing twin configuration (c.f. Figures 6.4, 6.5, 6.6). More precisely, there exists a universal constant $c > 0$ such that for any ball $B_r(x_0) \subset\subset \Omega$ the configuration in $B_{cr}(x_0)$ is either a simple laminate or a crossing twin configuration.

Rigidity statements of this form have been a topic of very active research in the last two decades. In particular, after the unexpected discovery of “wild” convex integration solutions by Müller & Šverák [MŠ99] a strong interest in rigidity properties of the underlying models developed. Starting with the work of Dolzmann & Müller [DM95a], [DM95b] on the two-well problem, such properties have been studied systematically, c.f. [Kir98], [Con08], [DKMŠ00a], [CDK07], [CO12]. For example, Dolzmann and Müller prove the following theorem for the cubic-to-tetragonal phase transition (which can, mathematically, be interpreted as a special case of the cubic-to-orthorhombic phase transition) in a geometrically linear framework:

Proposition 24 (Dolzmann & Müller, [DM95a]). *Let $\delta = 0$. Then any configuration of strains taking values in $\{e^{(1)}, \dots, e^{(6)}\}$ is locally a simple laminate.*

A central observation underlying all previously mentioned articles consists of noting that while the respective (nonlinear) n -well models can display convex integration solutions, models involving surface energy constraints do not. On the contrary, the above cited works have shown that under BV conditions strong rigidity properties hold.

As the first part of our discussion exemplifies, the cubic-to-orthorhombic phase transition displays such non-rigidity already in the geometrically *linearized* theory of elasticity. Therefore, a better understanding of conditions guaranteeing rigidity in this case seems desirable. Due to the large number of possible jump planes, such an analysis involves strong combinatorial elements already in the piecewise affine setting.

The proof of our result consists of two central elements:

- *Classification of zero-homogeneous strain configurations* (i.e. $e(\nabla u)(\lambda x) = e(\nabla u)(x)$). This corresponds to characterizing all possible three-dimensional corners involving strains of the cubic-to-orthorhombic phase transition. Here, we prove the following central proposition.

Proposition 25. *Let $\delta \notin \{\pm\frac{3}{2}, \pm 3\}$. Then any zero-homogeneous strain is given by a laminate or a crossing twin configuration (c.f. Figures 6.4, 6.5, 6.6).*

The classification of all homogeneous solutions can be considered as a necessary initial step in attaining a full understanding of configurations involving finite surface energy, i.e. piecewise polygonal structures and, in possible future work, also configurations involving BV constraints.

- *Combining zero-homogeneous corners.* As there are only finitely many jumps in piecewise polygonal configurations, these may be considered as combinations of only finitely many homogeneous corners which possibly yield a new, possibly more complex compatible structure.

Technically, the proof of our rigidity result consists of four key ingredients:

- *Regularity.* In a first step the strain equations are used in order to characterize homogeneous corners. We show that the “piecewise affine situation” is the correct one, i.e. strains can indeed only jump at planes determined by the piecewise affine compatibility conditions.
- *Blow-up procedure.* Instead of investigating the behaviour of a possible corner close to the origin, we “blow up” the corner. In three dimensions it is sufficient to understand the patterns which a corner induces on a sphere surrounding this corner, as compatibility amounts to a second order condition. Hence, if a configuration is compatible on the sphere, it is also compatible at the origin. (This would not be true in two dimensions as configurations which are compatible on the circle might still induce Dirac masses at the origin.)
- *Combinatorics on the sphere.* In a third step a Mathematica aided (symbolic) “brute force” computation combined with combinatorial considerations demonstrates that the only possible zero-homogeneous configurations are made up of laminates or crossing twins. An alternative approach without Mathematica computations is presented in the appendix. There we make extensive use of combinatorial considerations.
Combinatorial considerations for certain special lines (“invariant lines”) also play a central role in proof of the piecewise polygonal result, Proposition 23.
- *Strain equations.* In certain planes combinatorial arguments do not suffice. As, however, in this situation only *four* of the six strains have to be taken into account, we argue via the classical strain equations. In these planes we deduce rigidity.

The remaining part of the chapter is organized as follows: In Section 6.3 we recall various properties of strain tensors. Sections 6.4 and 6.5 treat zero-homogeneous strains. In a first step we derive regularity properties of zero-homogeneous strains (Section 6.4) and in a second step we carry out the necessary combinatorial considerations (Section 6.5). In Section 6.6 we address the piecewise polygonal situation. Last but not least, in the appendix, we give an additional computer-free, yet combinatorially more involved proof of the main rigidity result and briefly comment on the situation of $\delta \in \{\pm\frac{3}{2}, \pm 3\}$.

6.3 Preliminaries

Some Properties of Strains

We recall that a strain can be characterized by a Poincaré-like condition:

Lemma 17. *Let $U \subset \mathbb{R}^3$ be simply connected, $e : U \rightarrow \mathbb{R}_{sym}^{3 \times 3}$. Then the following are equivalent:*

- e is a strain corresponding to a deformation u ,
- e (distributionally) satisfies the strain equations

$$\nabla \times (\nabla \times e) = 0, \quad (6.3.1)$$

i.e. the following system of partial differential equations is satisfied distributionally:

$$\begin{aligned} \partial_{33}^2 e_{22} + \partial_{22}^2 e_{33} &= 2\partial_2 \partial_3 e_{23}, \\ \partial_{33}^2 e_{11} + \partial_{11}^2 e_{33} &= 2\partial_1 \partial_3 e_{13}, \\ \partial_{22}^2 e_{11} + \partial_{11}^2 e_{22} &= 2\partial_1 \partial_2 e_{12}, \end{aligned} \quad (6.3.2)$$

$$\begin{aligned} \partial_2 \partial_3 e_{11} &= \partial_1 (-\partial_1 e_{23} + \partial_2 e_{13} + \partial_3 e_{12}), \\ \partial_1 \partial_3 e_{22} &= \partial_2 (\partial_1 e_{23} - \partial_2 e_{13} + \partial_3 e_{12}), \\ \partial_1 \partial_2 e_{33} &= \partial_3 (\partial_1 e_{23} + \partial_2 e_{13} - \partial_3 e_{12}). \end{aligned} \quad (6.3.3)$$

Remark 25. As a strain tensor (six degrees of freedom) originates from a displacement field (three degrees of freedom) only three of the six equations are independent.

Proof of Lemma 17. As the first implication only amounts to a simple calculation, we only consider the second one. For that purpose we regard the vectorial formulation

$$\nabla \times (\nabla \times e) = 0.$$

Since U is simply connected, Poincaré's lemma implies

$$\nabla \times e = \nabla w \quad (6.3.4)$$

for a field $w : U \rightarrow \mathbb{R}^3$. Defining $\omega_{ij} := -\epsilon_{ijk}w_k$, we obtain

$$\begin{aligned} (\nabla \times \omega)_{ij} &= \epsilon_{ilk} \partial_l \omega_{jk} \\ &= -\epsilon_{ilk} \epsilon_{jks} \partial_l w_s \\ &= -\epsilon_{ilk} \epsilon_{jks} (\nabla \times e)_{sl} \\ &= -(\delta_{is} \delta_{lj} - \delta_{ij} \delta_{ls}) (\nabla \times e)_{sl} \\ &= -(\nabla \times e)_{ij}, \end{aligned}$$

where we exploited symmetry properties of the expressions involved. As a consequence, we have

$$0 = \nabla \times e + \nabla \times \omega.$$

Therefore, a second application of Poincaré's lemma yields the existence of a field $u : U \rightarrow \mathbb{R}^3$ satisfying

$$\nabla u = e + \omega.$$

The uniqueness of such a decomposition implies the claim. \square

As we will rely on various changes of coordinates, we briefly recall the transformation behaviour of strains. Being tensors of order two, they obey the following rule:

Lemma 18. *Let $e : \mathbb{R}^3 \rightarrow \mathbb{R}_{sym}^{3 \times 3}$ be a strain corresponding to a displacement field u . Let $C \in GL(3)$ and consider new coordinates given by*

$$\hat{x} = C^{-t}x, \quad \hat{u} = Cu.$$

Then the transformed strain $\hat{e}(\hat{\nabla}\hat{u})(\hat{x}) := \frac{\hat{\nabla}\hat{u}(\hat{x}) + (\hat{\nabla}\hat{u}(\hat{x}))^t}{2}$ can be derived from the original strain e :

$$\hat{e}(\hat{\nabla}\hat{u})(\hat{x}) = Ce(\nabla u)(x)C^t.$$

Polar Coordinates for Zero-Homogeneous Strains

Working with homogeneous strains, equation (6.3.1) can be rewritten as an equation on the sphere. For this purpose we use the following polar coordinates convention

$$x = \begin{pmatrix} r \cos(\varphi) \sin(\psi) \\ r \sin(\varphi) \sin(\psi) \\ r \cos(\psi) \end{pmatrix}, \quad \psi \in [0, \pi), \quad \varphi \in [0, 2\pi).$$

Hence, on the unit sphere the second derivatives for zero-homogeneous functions

turn into

$$\begin{aligned}
\frac{\partial^2}{\partial^2 x_1} &= \left(\frac{\sin(\varphi)}{\sin(\psi)} \frac{\partial}{\partial \varphi} - \cos(\varphi) \cos(\psi) \frac{\partial}{\partial \psi} + \cos(\varphi) \sin(\psi) \right) \\
&\quad \times \left(\frac{\sin(\varphi)}{\sin(\psi)} \frac{\partial}{\partial \varphi} - \cos(\varphi) \cos(\psi) \frac{\partial}{\partial \psi} \right), \\
\frac{\partial^2}{\partial^2 x_2} &= \left(\frac{\cos(\varphi)}{\sin(\psi)} \frac{\partial}{\partial \varphi} + \sin(\varphi) \cos(\psi) \frac{\partial}{\partial \psi} - \sin(\psi) \sin(\varphi) \right) \\
&\quad \times \left(\frac{\cos(\varphi)}{\sin(\psi)} \frac{\partial}{\partial \varphi} + \sin(\varphi) \cos(\psi) \frac{\partial}{\partial \psi} \right), \\
\frac{\partial^2}{\partial^2 x_3} &= \frac{\partial}{\partial \psi} \left(\sin^2(\psi) \frac{\partial}{\partial \psi} \right), \\
\frac{\partial^2}{\partial x_1 \partial x_2} &= \left(-\frac{\sin(\varphi)}{\sin(\psi)} \frac{\partial}{\partial \varphi} + \cos(\varphi) \cos(\psi) \frac{\partial}{\partial \psi} - \cos(\varphi) \sin(\psi) \right) \\
&\quad \times \left(\frac{\cos(\varphi)}{\sin(\psi)} \frac{\partial}{\partial \varphi} + \sin(\varphi) \cos(\psi) \frac{\partial}{\partial \psi} \right), \\
\frac{\partial^2}{\partial x_1 \partial x_3} &= \left(-\cos(\varphi) \cos(\psi) \frac{\partial}{\partial \psi} + \frac{\sin(\varphi)}{\sin(\psi)} \frac{\partial}{\partial \varphi} + \cos(\varphi) \sin(\psi) \right) \left(\sin(\psi) \frac{\partial}{\partial \psi} \right), \\
\frac{\partial^2}{\partial x_2 \partial x_3} &= \left(-\sin(\varphi) \cos(\psi) \frac{\partial}{\partial \psi} - \frac{\cos(\varphi)}{\sin(\psi)} \frac{\partial}{\partial \varphi} + \sin(\varphi) \sin(\psi) \right) \left(\sin(\psi) \frac{\partial}{\partial \psi} \right)
\end{aligned}$$

The difficulty of working directly with the strain equations on the sphere stems from the dependence on two independent variables, i.e. in contrast to toy models on one-dimensional spheres, we are confronted with a PDE instead of an ODE.

6.4 A Regularity Result

We now turn to proving the rigidity statement. As a first step, we give a justification of the “piecewise affine” picture for zero-homogeneous strains. For that purpose we deduce “one-dimensional conditions” from the strain equations.

More precisely, this step is achieved by considering the strain equations restricted to certain great circles on the sphere. On these, the equations turn into equations of a single variable from which it is possible to deduce additional regularity of the strains along these great circles. Carrying out a change of coordinates allows to conclude that similar equations hold on (almost) all great circles. Thus, via the regularity gain we can characterize all great circles on which jumps in the strains may occur. As a consequence, we derive the “piecewise affine” picture.

In order to carry out such an argument we need the following consequence of the coarea formula. This becomes necessary in order to show that there are sufficiently many “well-behaved” great circles.

Lemma 19. *Let $e \in L^\infty(\mathbb{S}^2; \mathbb{R}_{sym}^{3 \times 3})$ and let η_ϵ be a mollifier. Then for almost every great circle C we have convergence of the convolution $e^\epsilon := e * \eta_\epsilon$ restricted to this*

one-dimensional set:

$$e^\epsilon(x) \rightarrow e(x) \text{ as } \epsilon \rightarrow 0,$$

for \mathcal{H}^1 almost every $x \in C$.

With this statement we can derive one-dimensional compatibility conditions from the strain equations. Using our polar coordinates convention with $r = 1$, we have:

Lemma 20. *Let C be one of the following great circles:*

$$x(\cdot, \frac{\pi}{2}), x(0, \cdot), x(\pi, \cdot), x(\frac{\pi}{2}, \cdot), x(\frac{3\pi}{2}, \cdot).$$

Assume that $e \in L^\infty(C; \mathbb{R}_{sym}^{3 \times 3})$ and that $e^\epsilon|_C \rightarrow e|_C$ as $\epsilon \rightarrow 0$. Then the strain equations imply (depending on the respective great circle, one of) the conditions

$$\begin{aligned} \cos^2(\varphi)e_{11} + \sin^2(\varphi)e_{22} + 2\sin(\varphi)\cos(\varphi)e_{12} &\in W_\varphi^{1,\infty}, \\ \sin^2(\psi)e_{11} + 2\cos(\psi)\sin(\psi)e_{13} + \cos(\psi)e_{33} &\in W_\psi^{1,\infty}, \\ \sin^2(\psi)e_{11} - 2\cos(\psi)\sin(\psi)e_{13} + \cos(\psi)e_{33} &\in W_\psi^{1,\infty}, \\ \cos^2(\psi)e_{33} + \sin^2(\psi)e_{22} + 2\cos(\psi)\sin(\psi)e_{23} &\in W_\psi^{1,\infty}, \\ \cos^2(\psi)e_{33} + \sin^2(\psi)e_{22} - 2\cos(\psi)\sin(\psi)e_{23} &\in W_\psi^{1,\infty}, \end{aligned} \quad (6.4.1)$$

where $W_\psi^{1,\infty} := \{u \in L^\infty(\mathbb{S}^2) \mid u(\varphi, \cdot) \in W^{1,\infty}\}$ and $W_\varphi^{1,\infty}$ is defined analogously.

Remark 26. The different signs in the second and third as well as the fourth and fifth equation correspond to a rotation of $\frac{\pi}{2}$ with respect to the x_3 -axis.

Proof. We consider the first equation, i.e. the equation for the angle

$$\psi = \frac{\pi}{2}.$$

The heuristic idea of the proof consists of considering the strain equation on the given great circle. Under the assumption of a sufficiently regular strain, we may restrict the strain equation onto this great circle:

$$\sin^2(\varphi)\frac{\partial}{\partial\varphi}e_{22} + \cos^2(\varphi)\frac{\partial}{\partial\varphi}e_{11} + 2\sin(\varphi)\cos(\varphi)\frac{\partial}{\partial\varphi}e_{12} = 0.$$

Commuting the derivatives with the functions of φ , yields

$$\frac{\partial}{\partial\varphi}(\sin^2(\varphi)e_{22} + \cos^2(\varphi)e_{11} + 2\sin(\varphi)\cos(\varphi)e_{12}) \in L^\infty,$$

which implies that as a function of φ

$$\sin^2(\varphi)e_{22} + \cos^2(\varphi)e_{11} + 2\sin(\varphi)\cos(\varphi)e_{12} \in W_\varphi^{1,\infty}.$$

In order to make this argument rigorous we use convolution and the assumed con-

vergence properties of the convolved strains. In fact we have

$$\frac{\partial}{\partial \varphi}(\sin^2(\varphi)e_{22}^\epsilon + \cos^2(\varphi)e_{11}^\epsilon + 2\sin(\varphi)\cos(\varphi)e_{12}^\epsilon) = P(\sin(\varphi), \cos(\varphi), e^\epsilon) \in L^\infty,$$

where P is a linear expression in the strain.

We formulate this as a distributional equality

$$\begin{aligned} - \int_C (\sin^2(\varphi)e_{22}^\epsilon + \cos^2(\varphi)e_{11}^\epsilon + 2\sin(\varphi)\cos(\varphi)e_{12}^\epsilon) \frac{\partial}{\partial \varphi} \zeta d\varphi \\ = \int_C \zeta P(\sin(\varphi), \cos(\varphi), e^\epsilon) d\varphi. \end{aligned}$$

Passing to the limit $\epsilon \rightarrow 0$ leads to

$$\begin{aligned} - \int_C (\sin^2(\varphi)e_{22} + \cos^2(\varphi)e_{11} + 2\sin(\varphi)\cos(\varphi)e_{12}) \frac{\partial}{\partial \varphi} \zeta d\varphi \\ = \int_C \zeta P(\sin(\varphi), \cos(\varphi), e) d\varphi. \end{aligned}$$

Hence, we conclude

$$\sin^2(\varphi)e_{22} + \cos^2(\varphi)e_{11} + 2\sin(\varphi)\cos(\varphi)e_{12} \in W_\varphi^{1,\infty}(C)$$

for $\psi = \frac{\pi}{2}$. The remaining equations can be derived analogously. \square

Remark 27. Due to Lemma 19, the assumptions on the convergence of the strains on the specified great circles can always be achieved after an appropriate change of coordinates.

In the sequel we extend the one-dimensional equations obtained above to equations on the whole sphere. For this purpose we carry out a change of coordinates which transforms a given great circle into one of the special great circles of Lemma 20.

We only consider the first equation in (6.4.1) for the moment. Changing coordi-

nates with a constant rotation matrix $P(\psi) = \begin{pmatrix} \cos(\psi) & 0 & -\sin(\psi) \\ 0 & 1 & 0 \\ \sin(\psi) & 0 & \cos(\psi) \end{pmatrix}$ the equation

remains valid:

Lemma 21. Let $v(\varphi, \psi) = P(\psi) \begin{pmatrix} \cos(\varphi) \\ \sin(\varphi) \\ 0 \end{pmatrix}$ and $\hat{e}(\hat{x}) = P(\psi)^t e(v(\varphi, \psi)) P(\psi)$.

Then (6.4.1) holds true for \mathcal{H}^1 a.e. choice of $\psi \in [0, \pi]$:

$$f(\varphi, \hat{e}(\varphi, \psi)) := \sin^2(\varphi)\hat{e}_{22} + \cos^2(\varphi)\hat{e}_{11} + 2\sin(\varphi)\cos(\varphi)\hat{e}_{12} \in W_\varphi^{1,\infty}.$$

This can be rephrased as

$$\begin{pmatrix} \cos(\varphi) \\ \sin(\varphi) \\ 0 \end{pmatrix} P(\psi)^t \cdot e(v(\varphi, \psi)) P(\psi) \begin{pmatrix} \cos(\varphi) \\ \sin(\varphi) \\ 0 \end{pmatrix} = v(\varphi, \psi) \cdot e(v(\varphi, \psi)) \quad v(\varphi, \psi) \in W_\varphi^{1,\infty}. \quad (6.4.2)$$

Remark 28. Heuristically speaking, Lemma 21 illustrates that we may assume (6.4.1) to be valid on the whole sphere. In particular, it demonstrates the usefulness of frame indifference.

Proof. After an appropriate change of coordinates (6.4.1) holds on $\psi = \frac{\pi}{2}$. Thus, we carry out the change of coordinates (determined by $P^t(\psi)$)

$$P(\psi) \begin{pmatrix} \cos(\varphi) \\ \sin(\varphi) \\ 0 \end{pmatrix} \mapsto \begin{pmatrix} \cos(\varphi) \\ \sin(\varphi) \\ 0 \end{pmatrix}.$$

Applying the transformation formula for strains yields the desired result. \square

Finally, the ‘‘piecewise affine’’ picture can be justified by combining the previously derived results.

Lemma 22. *Let $e_1, \dots, e_6 \in \mathbb{R}_{sym}^{3 \times 3}$ be such that there exist $a_{ij} \in \mathbb{R}^3 \setminus \{0\}, n_{ij} \in \mathbb{S}^2$ with $e_i - e_j = \frac{1}{2}(a_{ij} \otimes n_{ij} + n_{ij} \otimes a_{ij})$. Then zero-homogeneous solutions of the strain equations are piecewise affine and jumps in the strains can only occur at planes with normals given by a_{ij} or n_{ij} .*

Proof. Let $\psi \in [0, \pi)$ be arbitrary but fixed. Using the notation introduced in the previous lemma, we are interested in finding possible values of φ for which $e(\nabla u)$ may jump from one strain, e_i , to another one, e_j , on the great circle parametrized by $v(\varphi, \psi)$. As $f(\varphi, \hat{e}(\varphi, \psi))$ is a $W^{1,\infty}$ function of φ , a jump from strain e_i to strain e_j can only occur at an angle φ_0 if

$$f(\varphi_0, \hat{e}_i(\varphi_0, \psi)) = f(\varphi_0, \hat{e}_j(\varphi_0, \psi)). \quad (6.4.3)$$

Thus, in order to find the points on a given great circle on which the strains can jump, it suffices to use (6.4.3) to calculate φ_0 as a function of ψ and of arbitrary strain configurations.

Recalling (6.4.2) and $\dim(e_i - e_j) \leq 2$, equation (6.4.3) reads

$$\begin{aligned} 0 &= v(\varphi, \psi) \cdot (e_i - e_j)v(\varphi, \psi) = \frac{1}{2}v(\varphi, \psi) \cdot (a_{ij} \otimes n_{ij} + n_{ij} \otimes a_{ij})v(\varphi, \psi) \\ &= (a_{ij} \cdot v)(n_{ij} \cdot v). \end{aligned}$$

This implies that jumps can only occur at angles φ_0 with

$$a_{ij} \cdot v(\varphi_0, \psi) = 0 \text{ or } n_{ij} \cdot v(\varphi_0, \psi) = 0.$$

Combining this with the other equations in (6.4.1), yields the claim (it is in fact necessary to use the other equations as well, since the previous Lemma only guarantees the validity of the equations on almost every great circle). \square

6.5 Combinatorics on the Sphere

In this section we present the second key ingredient of the rigidity proof for zero-homogeneous configurations. This includes (symbolic) Mathematica computations and a combinatorial argument showing that the configurations cannot be more complex than the crossing twin structures. (A Mathematica-free proof involves slightly more combinatorics and is postponed to the appendix.)

We make use of two central elements.

- *Local combinatorics.* Firstly, we calculate – with a symbolic calculation in Mathematica – all possible intersections of the jump planes/ jump great circles on the sphere, saving the respective points, normals and strain variants involved. This yields a two-dimensional situation in which it becomes possible to determine all compatible configurations by checking simple compatibility conditions. Thus, Mathematica calculations characterize all spherical points at which two-dimensional corners can occur.
- *Global combinatorics.* In the second step it remains to combine the local information into global structures on the sphere. This is carried out “by hand” by checking all possible patterns on a graph on the sphere.

Before discussing the situation on the sphere, we recall the following compatibility condition.

Lemma 23. *Let $e_1, \dots, e_n \in \mathbb{R}_{sym}^{3 \times 3}$ and assume that there exist vectors $a_{ij} \in \mathbb{R}^3 \setminus \{0\}$, $n_{ij} \in \mathbb{S}^2$ such that*

$$e_i - e_j = \frac{1}{2}(a_{ij} \otimes n_{ij} + n_{ij} \otimes a_{ij}) \text{ for } i \neq j.$$

Assume that there exists a point at which m of these strains form a corner. Then turning once around the corner, it holds

$$\sum_{k=1}^m a_{i_k j_k} \otimes n_{i_k j_k} = 0.$$

Remark 29. In the formulation of the lemma we keep track of the orientation, i.e. while the normal and shear corresponding to a jump from e_i to e_j is given by n_{ij} , a_{ij} the normal and shear for a jump from e_j to e_i is given by $n_{ji} = -n_{ij}$, $a_{ji} = a_{ij}$.

Proof. This follows from the fact that in order to have a compatible corner not only the symmetric parts of the strain, but also its antisymmetric parts have to “fit”, i.e. turning once around the corner, one has to arrive at the initial skew symmetric matrix. \square

We begin by characterizing all possible intersection points of different phases on the sphere. At this stage we make use of symbolic Mathematica computations in order to obtain the intersection points, and to subsequently derive all admissible corners.

When speaking about intersection points, it will be convenient to use the notion of degree. Therefore, we introduce the following definition.

Definition 9. *A point $x \in \mathbb{S}^2$ is a corner of degree n or an n -fold corner if in an arbitrarily small neighbourhood of x there are n (not necessarily pairwise different) strain variants separated by great circle segments such that neighbouring strains are pairwise different.*

Excluding the cases $\delta \in \{\pm\frac{3}{2}, \pm 3\}$ (which are briefly discussed in the appendix), we have:

Lemma 24. *Let $e \in \{e^{(1)}, \dots, e^{(6)}\}$ and $\delta \notin \{\pm\frac{3}{2}, \pm 3\}$. Then there are only corners of degree two (which locally correspond to twin configurations) or of degree four on the sphere. The corners of degree four can only occur at the points*

$$(1, 0, 0), (0, 1, 0), (0, 0, 1), \left(\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right), \left(\frac{1}{\sqrt{2}}, 0, -\frac{1}{\sqrt{2}}\right), \left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right), \left(\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}, 0\right), \\ (0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}), (0, \frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}),$$

and at their respective antipodal points. A schematic overview of all possible corners is given in Figures 6.4, 6.5, 6.6.

Proof of Lemma 24. The lemma follows from a Mathematica computation: In a first step we compute all possible points of intersection of the various jump planes. Secondly, we compute the possible configurations at these points. As at most four planes intersect at a given point, this yields an upper bound on the degree of the corner – the degree is at most 8. Then the admissible corners are found by checking the (oriented) compatibility condition

$$\sum_{k=1}^m n_{i_k j_k} \otimes a_{i_k j_k} = 0.$$

\square

The characterization of the possible corners allows to combine the local information, i.e. the possibility of forming corners, with the global structures on the sphere. This is achieved via a “brute force” argument successively considering all possible combinations of jumps. Fortunately, this reduces to understanding the behaviour

of the strains at the four-fold corners; thus the necessary combinatorial effort is limited.

Proof of Proposition 25. It suffices to prove the statement at the points $(1, 0, 0)$ and $(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$, as the other points can then be obtained by a rotation of the coordinates (which coincides with symmetries of the strains). For these two points we argue combinatorially, i.e. we start with a four-fold corner at the given point and show that any configuration resulting from this has to be a crossing twin structure. In the sequel we will make extensive use of the following claim.

Claim 1. *Starting from a given four-fold corner, the configuration remains unchanged until the next corner at which a possible four-fold corner can occur is reached. More precisely, for each edge of the currently considered configuration there is a neighbourhood such that the configuration remains constant until the next possible corner is reached.*

Proof of Claim 1. We show that if this were not the case, another four-fold corner would exist prior to the next corner: This follows from the fact, that, on the one hand, there is only a finite number of corners. On the other hand, any change of configuration not occurring at one of the admissible corners of degree four would create a corner of degree at least three on one of the edges, which is impossible before reaching the next admissible corner. \square

The argument excluding structures different from crossing twins consists of successively considering all possible configurations starting from a given one and proving that, apart from the initially chosen four-fold corner, the only further compatible corner of degree four is the antipodal point of the initial corner. In the sequel we carry out the argument for $\delta \notin \{\pm\frac{3}{2}, \pm 3\}$.

Step 1: Configurations at $(1, 0, 0)$ involving K3.

We begin with the configuration K3 at $(1, 0, 0)$ (in Figure 6.4 this corresponds to the third configuration). We remark that the schematic notation of Figure 6.4 actually corresponds to four different configurations (c.f. Figure 6.2), K3a - K3d.

By symmetry it suffices to consider the first two configurations, K3a, K3b. The phase arrangement of K3c and K3d can be obtained from these by a rotation by 180° . Due to the observation contained in Claim 1, it suffices to exclude a change in the configuration at the next four-fold corner. Thus, step by step, we check compatibility at the vertices of the graph which is made up of the points at which possible corners of degree four are located.

Before going through the individual vertices on the spherical graph, we point out the following observation:

Observation 1. *For both configurations K3a, K3b, the great circle passing through the points $(1, 0, 0)$, $(0, -\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$ always remains a phase interface, i.e. it always separates two non-equal phases.*

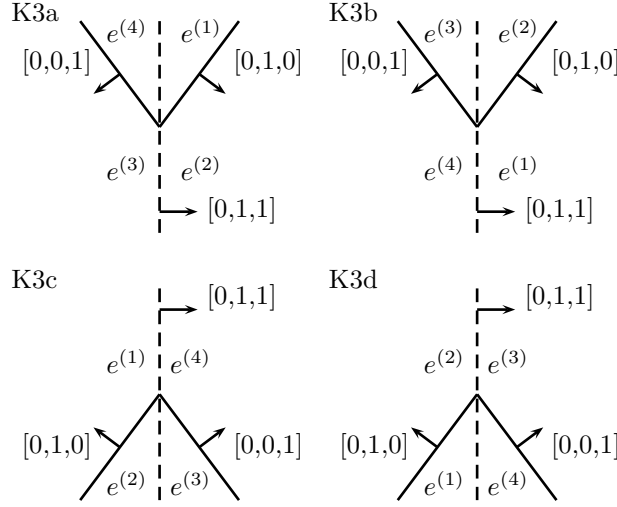


Figure 6.2: Possible configurations K3a-K3d.

Proof of Observation 1. In order to understand this, we consider the possible changes of the initial configuration at the points $(0, -\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$ and $(0, \frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}})$. As the configuration at $(0, -\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$ has to contain a direct interface between the strains $e^{(1)}$ and $e^{(4)}$ in case of K3a and a direct interface between $e^{(2)}$ and $e^{(3)}$ in case of K3b, this implies that at this point either no change occurs or the configuration changes to K2. In both cases the great circle with normal $[0, 1, 1]$ remains an interface. At $(0, \frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}})$ an analogous argument shows that the configuration either remains unchanged or changes but preserves the phase interface determined by the normal $[0, 1, 1]$. Hence, the claim follows. \square

With this observation, we investigate the situation on the spherical graph. It is possible to deal with the cases K3a and K3b simultaneously:

- $(-\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}, 0)$: Here possible configurations are provided by K13 and K14. K13 can be excluded immediately as in this configuration $e^{(3)}$ and $e^{(4)}$ are not neighbouring strains. K14 cannot be realized as this would cause a non-admissible corner on the great circle passing through $(1, 0, 0)$ and $(0, -\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$ if $\delta \notin \{\pm\frac{3}{2}, \pm 3\}$.
- $(\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}})$: At this point the possible configurations are K11 and K12. As above K11 can be excluded due to the arrangement of neighbouring strains. In order to be compatible, we would need a corner in which $e^{(1)}$ and $e^{(2)}$ constitute neighbouring strains. Due to $\delta \notin \{\pm\frac{3}{2}, \pm 3\}$, configuration K12 cannot occur as this would involve a non-admissible corner on the great circle connecting $(1, 0, 0)$ and $(0, -\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$.
- $(0, -1, 0)$, $(0, 0, 1)$: At these points the configuration remains unchanged as the configurations K9, K10 at $(0, 1, 0)$ do not involve $e^{(4)}$ and K15, K16, as the possible configurations at $(0, 0, 1)$, do not involve $e^{(1)}$.

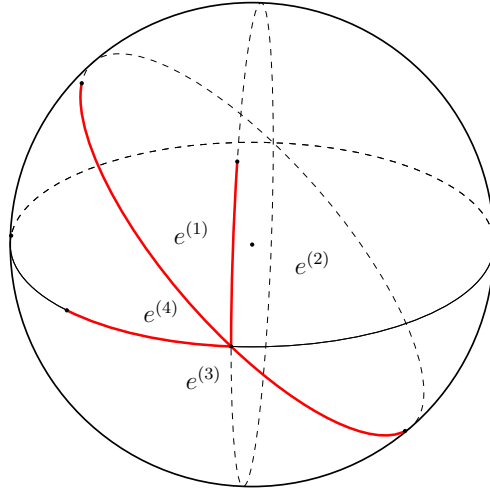


Figure 6.3: The configuration K3a on the sphere.

- $(-\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}, 0)$: On the one hand, configuration K17 can be excluded as there is no interface connecting $e^{(3)}$ and $e^{(4)}$. On the other hand, K18 would produce a non-admissible corner on the great circle passing through $(-1, 0, 0)$ and $(0, \frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}})$.
- $(-\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}})$: Here, configuration K7 can be excluded immediately as it does not contain a direct interface between $e^{(1)}$ and $e^{(2)}$. As in the previous considerations, configuration K8 would entail a non-admissible corner on the great circle passing through $(-1, 0, 0)$ and $(0, \frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}})$.

As a consequence, we deduce that at $(-1, 0, 0)$ the configuration has to coincide with K3, i.e. there are no changes in the configuration at $(0, -\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$. Furthermore, this implies that the configuration also remains unchanged at $(0, \frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}})$. Also, no changes in the configuration are possible at $(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$ or at $(-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$ since the configurations at these points neither involve the strain $e^{(1)}$ nor $e^{(2)}$. Therefore, the configuration is stable at $(0, 1, 0)$ and $(0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$ as well. An analogous argument shows that there are no changes at $(\frac{1}{\sqrt{2}}, 0, -\frac{1}{\sqrt{2}})$, $(-\frac{1}{\sqrt{2}}, 0, -\frac{1}{\sqrt{2}})$, $(0, -\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}})$ and at $(0, 0, -1)$. Hence, the configuration is given by the expected, simple four-fold corner.

Step 2: Configurations at $(1, 0, 0)$ involving K4.

We consider the initial strain distribution given by K4. As in Step 1, we note that the “diagonal” great circle remains an interface independent of possible changes in the configuration. As above, we follow the possible four-fold corners for the configurations K4a, K4b:

- $(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$: K17 can be excluded as there is no direct interface between $e^{(3)}$ and $e^{(4)}$. The second configuration, K18, causes a non-admissible corner on

the great circle connecting $(1, 0, 0)$ and $(0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$ for $\delta \notin \{\pm\frac{3}{2}, \pm 3\}$.

- $(\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}})$: On the one hand, K11 is incompatible as there is no neighbouring connection between $e^{(1)}$ and $e^{(2)}$. On the other hand, K12 would imply a non-admissible corner on the great circle joining $(1, 0, 0)$ and $(0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$ if $\delta \notin \{\pm\frac{3}{2}, \pm 3\}$.
- $(0, 1, 0), (0, 0, 1)$: These configurations are both incompatible as K9 and K10 do not include $e^{(3)}$ and $e^{(4)}$ and as K15 and K16 do not involve $e^{(1)}$ and $e^{(2)}$.
- $(0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$: The configuration K6 is not admissible since it does not contain a direct interface between $e^{(1)}$ and $e^{(3)}$. The second possibility, K5, can be excluded since it would cause a non-admissible corner on the great circle joining $(1, 0, 0)$ and $(0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$.
- $(-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$: Again, configuration K13 cannot occur as this configuration does not involve a direct interface between $e^{(3)}$ and $e^{(4)}$. K14 would cause a non-admissible corner on the great circle passing through $(0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$ and $(-1, 0, 0)$.

As in step 1 this suffices to deduce that at $(-1, 0, 0)$ the only compatible configuration coincides with the initially chosen four-fold corner K4. Furthermore, the same arguments as above imply that there cannot be any changes of this configuration.

Step 3: Four-fold configurations at $(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$.

At this point the various versions of configurations K17 and K18 represent possible four-fold corners:

- All initial configurations include the normals $[3, -3, -2\delta], [3, -3, 2\delta]$. If $\delta \notin \{\pm\frac{3}{2}, \pm 3\}$ then the great circles corresponding to these normals do not contain any admissible corners except the starting point, $(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$, and its antipodal point, $(-\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}, 0)$. Hence, the configuration along both great circles is not changed until the antipodal point is reached. As this holds for both great circles, the configuration at the antipodal point has to coincide with the one at the starting point. In effect, the whole great circle segments which are determined by the normals $[3, -3, -2\delta], [3, -3, 2\delta]$ must be phase interfaces.
- Due to the considerations carried out at the point $(1, 0, 0)$, there cannot be a change of the configuration at any of the points $\pm(1, 0, 0), \pm(0, 1, 0), \pm(0, 0, 1)$ as else this would have appeared in the analysis of the configurations at $(1, 0, 0)$.
- At the remaining points $\pm(\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}), \pm(-\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}), \pm(0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}), \pm(0, -\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}), \pm(-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$, no changes can occur, as any of the admissible configurations at these points contains normals which are of the form $[\pm 3, \pm 3, \pm 2\delta]$ (and permutations thereof). Since these great circles do not

intersect any other admissible corner except the one antipodal to the starting configuration, this necessarily leads to a non-admissible intersection point with the great circles determined by the normals $[3, -3, -2\delta]$, $[3, -3, 2\delta]$ if $\delta \notin \{\pm\frac{3}{2}, \pm 3\}$.

This proves the claim. \square

6.6 Piecewise Affine Strains

Due to the previous results on zero-homogeneous configurations, it is possible to tackle the piecewise polygonal situation without any homogeneity assumption for the full six-well problem. In this setting we deal with structures involving an arbitrary but finite number of jumps. These can also be characterized as piecewise affine configurations according to Liouville's theorem. Arguing via the classification of the homogeneous strains, further combinatorial considerations and the classical strain equations, we deduce that – like in the homogeneous case – the most involved configurations locally consist of crossing twin structures in piecewise affine arrangements of strains:

Proposition 23. *Let $\delta \notin \{\pm\frac{3}{2}, \pm 3\}$. Assume that $\Omega \subset \mathbb{R}^3$ is a Lipschitz domain. Then any piecewise polygonal strain with*

$$e(\nabla u) \in \{e^{(1)}, \dots, e^{(6)}\} \text{ in } \Omega,$$

is locally either given by a laminate or a crossing twin configuration (c.f. Figures 6.4, 6.5, 6.6). More precisely, there exists a universal constant $c > 0$ such that for any ball $B_r(x_0) \subset\subset \Omega$ the configuration in $B_{cr}(x_0)$ is either a simple laminate or a crossing twin configuration.

Such a result can only be proven locally since boundary effects cannot, in general, be neglected. This means that in bounded domains there might be configurations that do not correspond to simple laminates or crossing twins as the incompatible corners are avoided by first hitting the boundary. In the sequel, we investigate the following class of configurations:

Definition 10. *A piecewise polygonal configuration of strains is an arrangement of a finite number of strains such that*

- *the strains are locally constant,*
- *the domains with constant strains are polygons,*
- *for each strain variant there are only a finite number of different connected components.*

Remark 30. Similar definitions can be used in the periodic and whole space setting.

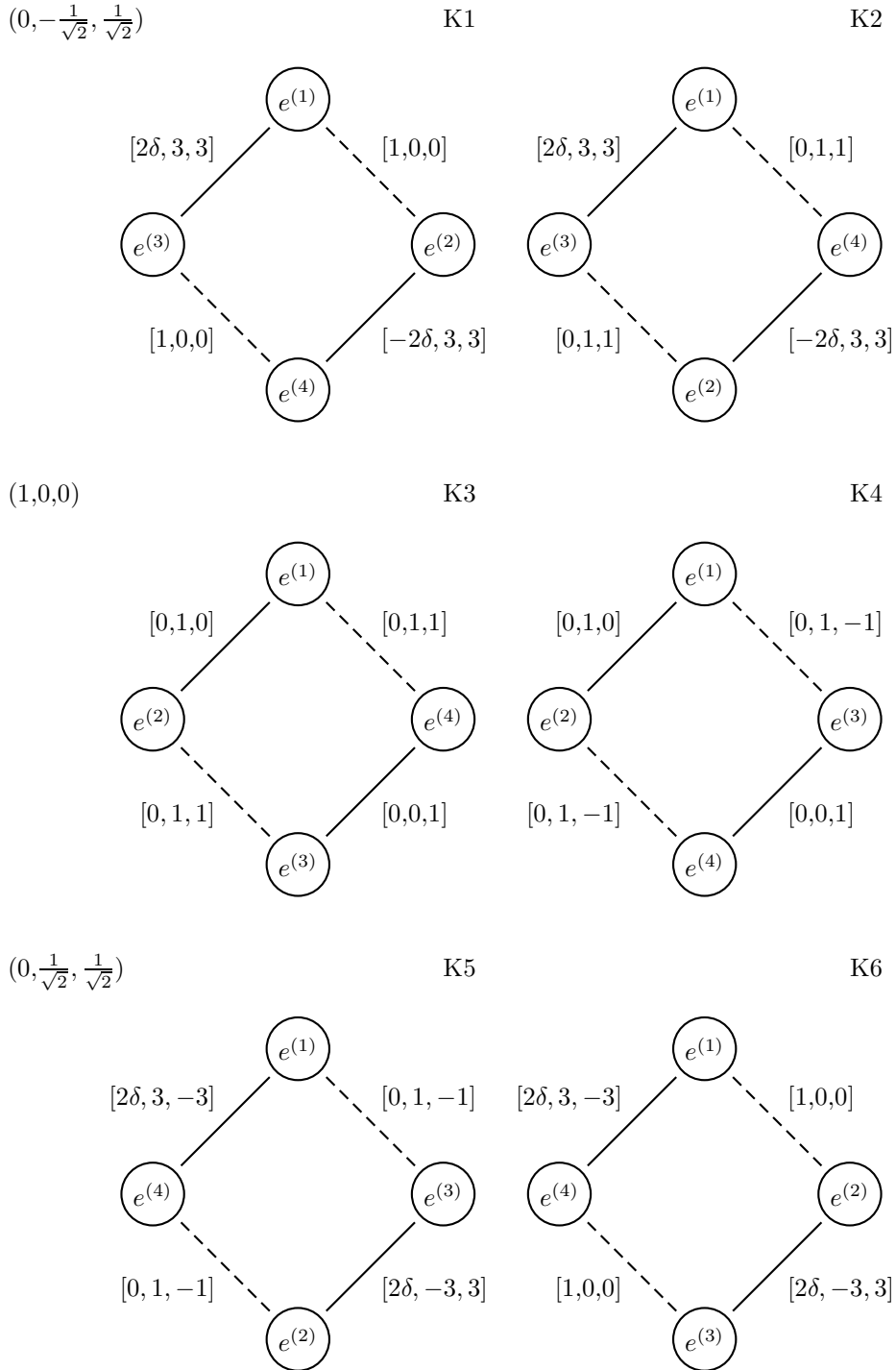


Figure 6.4: Compatible corners involving the strains $e^{(1)}, e^{(2)}, e^{(3)}, e^{(4)}$. The dashed lines depict the outer twins while the straight lines represent the “zig-zag bands” of the inner twins.

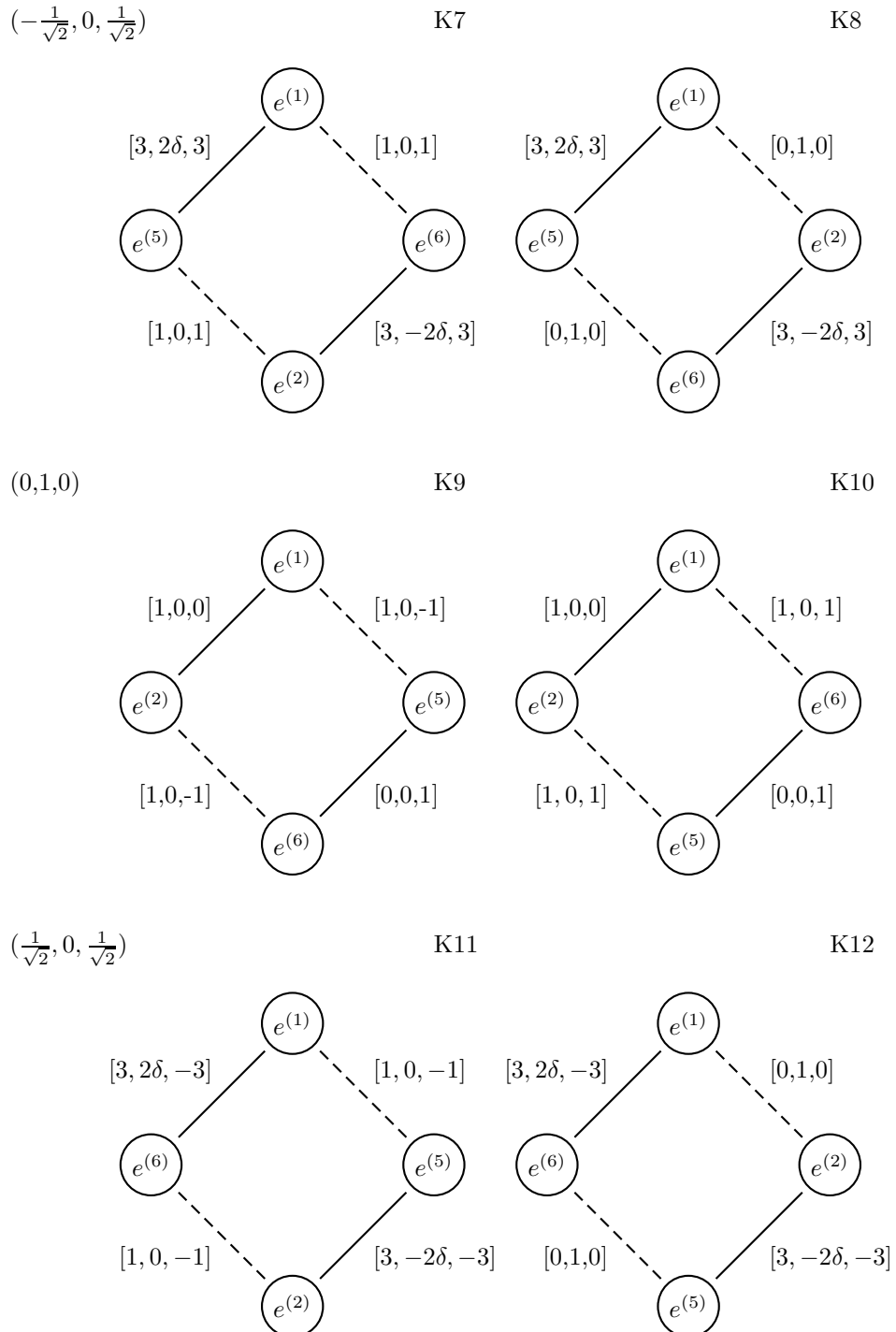


Figure 6.5: Compatible corners involving the strains $e^{(1)}, e^{(2)}, e^{(5)}, e^{(6)}$.

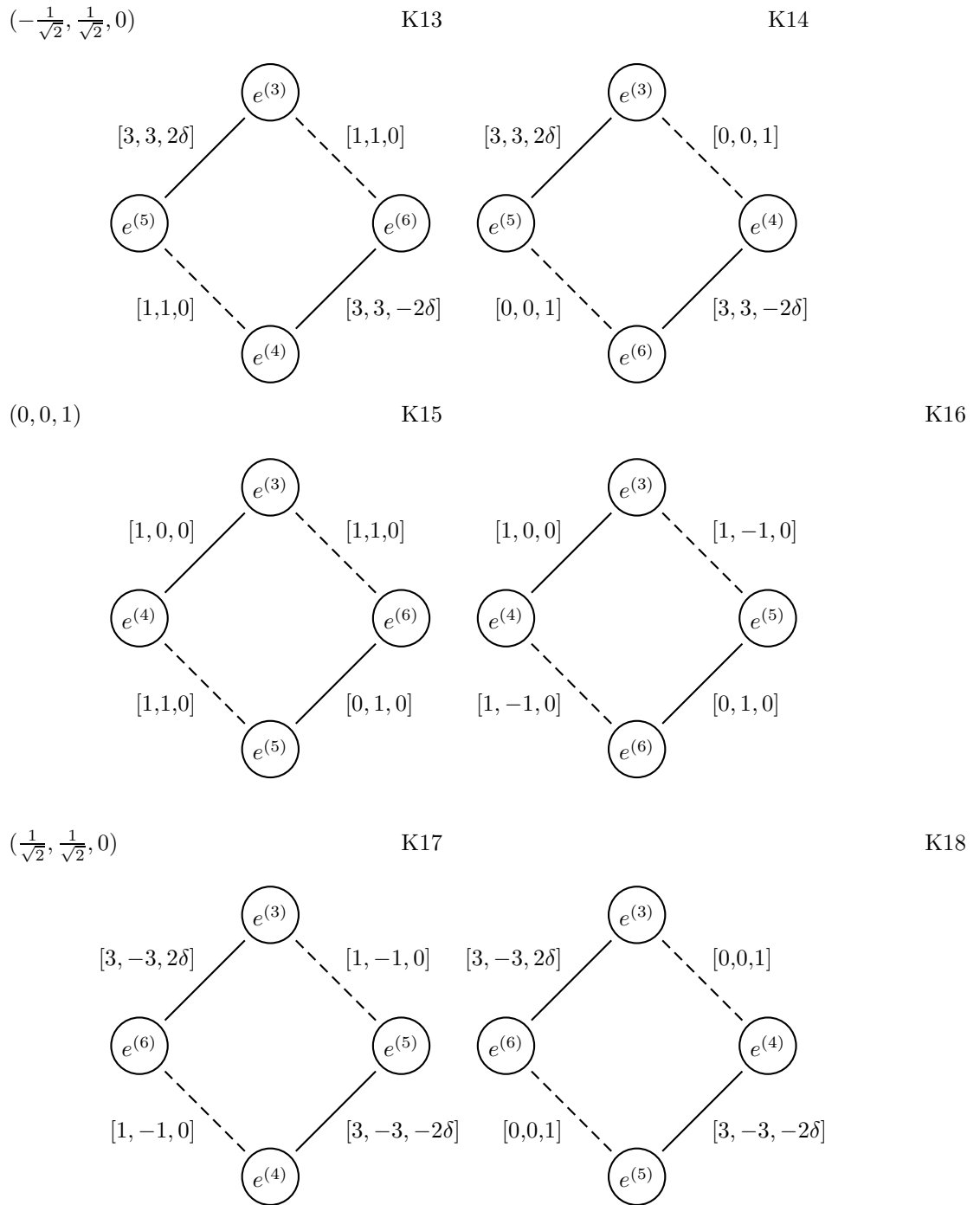


Figure 6.6: Compatible strains involving $e^{(3)}, e^{(4)}, e^{(5)}, e^{(6)}$.

We first consider certain planar configurations of strains. In the proof of Proposition 23 these cannot be dealt with in a purely combinatorial manner. Instead, the particular planar dependence of the strains allows for an analytic approach. The configurations under consideration correspond to “parallel invariant lines” (c.f. Observation 2).

In a second step we establish rigidity for “transversal invariant lines”. For these we argue combinatorially.

Planar Configurations

In the sequel we demonstrate that in specific planes any configuration of martensite variants consists of at most crossing twins. The key ingredients are based on characterizing strain tensors which only depend on the respective planar variables, exploiting the discrete structure of the components of the strains, and on employing the right change of coordinates. A similar version of this two-dimensional argument already appeared in [Rül10].

As will become clear from the proof of Proposition 23, we only need to consider configurations of *four* strains depending on *two* variables which are in a plane orthogonal to one of the following vectors:

$$\begin{aligned} & [1, 0, 0], [0, 1, 1], [0, -1, 1] \text{ and the strains } e^{(1)}, e^{(2)}, e^{(3)}, e^{(4)}; \\ & [0, 1, 0], [1, 0, 1], [1, 0, -1] \text{ and the strains } e^{(1)}, e^{(2)}, e^{(5)}, e^{(6)}; \\ & [0, 0, 1], [1, 1, 0], [1, -1, 0] \text{ and the strains } e^{(3)}, e^{(4)}, e^{(5)}, e^{(6)}. \end{aligned}$$

However, we prove a slightly stronger statement involving six strains in the planes described above.

In this planar setting it proves to be advantageous to carry out a change of coordinates and to renormalize the strains. As all the strains are symmetry related, it suffices to consider the first case, i.e. the respective planes are normal to one of the vectors $[1, 0, 0]$, $[0, 1, 1]$, $[0, -1, 1]$. This suggests to use the following change of coordinates which consists of a rotation combined with a renormalization step: We define $y = Cx$, with

$$C = \sqrt{3}\delta \begin{pmatrix} 0 & 1 & 1 \\ \sqrt{2} & 0 & 0 \\ 0 & 1 & -1 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{3}} & 0 & 0 \\ 0 & \frac{\sqrt{3}}{\sqrt{2}\delta} & 0 \\ 0 & 0 & \frac{1}{\sqrt{3}} \end{pmatrix}.$$

Correspondingly, the strains transform according to Lemma 18. As a result, we are

left with the following strain matrices

$$\begin{aligned}\tilde{e}^{(1)} &= \frac{1}{2d} \begin{pmatrix} d_1 & 1 & 1 \\ 1 & d_2 & 1 \\ 1 & 1 & d_3 \end{pmatrix}, \quad \tilde{e}^{(2)} = \frac{1}{2d} \begin{pmatrix} d_1 & -1 & 1 \\ -1 & d_2 & -1 \\ 1 & -1 & d_3 \end{pmatrix}, \\ \tilde{e}^{(3)} &= \frac{1}{2d} \begin{pmatrix} d_1 & 1 & -1 \\ 1 & d_2 & -1 \\ -1 & -1 & d_3 \end{pmatrix}, \quad \tilde{e}^{(4)} = \frac{1}{2d} \begin{pmatrix} d_1 & -1 & -1 \\ -1 & d_2 & 1 \\ -1 & 1 & d_3 \end{pmatrix}, \\ \tilde{e}^{(5)} &= \frac{1}{2d} \begin{pmatrix} \frac{2+2\delta}{3} & 0 & 0 \\ 0 & -\frac{6}{\delta^2} & 0 \\ 0 & 0 & \frac{2-2\delta}{3} \end{pmatrix}, \quad \tilde{e}^{(6)} = \frac{1}{2d} \begin{pmatrix} \frac{2-2\delta}{3} & 0 & 0 \\ 0 & -\frac{6}{\delta^2} & 0 \\ 0 & 0 & \frac{2+2\delta}{3} \end{pmatrix},\end{aligned}$$

where $d^{-1} = 6\delta^2$, $d_1 = -\frac{1}{3}$, $d_2 = \frac{3}{2\delta^2}$, $d_3 = -\frac{1}{3}$. In the sequel we will suppress the tildes in the notation.

Again, due to symmetry considerations, it suffices to consider strains which only depend on the first two variables. With a slight abuse of notation, we also denote these by $e = e(y_1, y_2)$ in the sequel. For these we prove the following:

Proposition 26. *Let $U \subset \mathbb{R}^3$ be open, convex, $\delta \notin \{\pm\frac{3}{2}, \pm 3\}$. Assume $e(\nabla u) : U \rightarrow \mathbb{R}_{sym}^{3 \times 3}$, $e(\nabla u) = e(y_1, y_2) = \frac{\nabla u + (\nabla u)^t}{2}$, $u \in W^{1,\infty}(U, \mathbb{R}^3)$ such that*

$$e(\nabla u) \in \{e^{(1)}, e^{(2)}, e^{(3)}, e^{(4)}, e^{(5)}, e^{(6)}\}$$

in U . Then the following statements hold:

1. *Either $e(\nabla u) \in \{e^{(1)}, \dots, e^{(4)}\}$ or $e(\nabla u) \in \{e^{(5)}, e^{(6)}\}$, in particular the second case implies that locally only simple laminates occur.*
2. *If $e(\nabla u) \in \{e^{(1)}, \dots, e^{(4)}\}$, then the following dichotomy holds:*

$$e_{12} = e_{12}(y_1) \quad \text{or} \quad e_{12} = e_{12}(y_2).$$

3. *In the case $e_{12} = e_{12}(y_1)$ there exists a function $g(t)$ such that:*

$$(e_{13} \circ \Phi)(s, t) = e_{12}(s)g(t) \quad \text{and} \quad (e_{23} \circ \Phi)(s, t) = g(t),$$

$$\text{where } \Phi(s, t) = (s, -E_{12}(s) + t) \text{ and } E'_{12}(y_1) = e_{12}(y_1), \quad E_{12}(0) = 0.$$

Due to symmetry, $e = e(y_1, y_2)$ can also be replaced by $e(y_1, y_3)$ and $e(y_2, y_3)$ respectively which yields analogous results. Furthermore, the case $e_{12} = e_{12}(y_2)$ can be treated analogously.

Proposition 26 corresponds to a rigidity result: Two-dimensional martensitic structures consist at most of crossing twins in the respective planes.

Remark 31. The statement of the theorem remains true if $\delta \in \{\pm\frac{3}{2}, \pm 3\}$ and if one only allows (up to permutations)

$$e(\nabla u) \in \{e^{(1)}, e^{(2)}, e^{(3)}, e^{(4)}\}.$$

As a crucial ingredient of the proof of the rigidity result, we observe that the strain equations (6.3.2), (6.3.3) simplify for the two-dimensional strains under consideration. Due to the planar dependence of the strains, $e = e(y_1, y_2)$, the system (6.3.2) of strain compatibility equations decouples into two equations for e_{33} and an equation coupling e_{11} , e_{22} , e_{12} :

$$\begin{aligned}\partial_{11}e_{33} &= 0, \\ \partial_{22}e_{33} &= 0, \\ \partial_{11}e_{22} + \partial_{22}e_{11} &= 2\partial_1\partial_2e_{12}.\end{aligned}$$

Due to the y_3 -independence of the strain and the discreteness of the values attained by e_{33} this, in particular, implies $e_{33} = \text{const}$. However, if $\delta \notin \{\pm\frac{3}{2}, \pm 3\}$, this can only be the case if $e(\nabla u) \in \{e^{(1)}, e^{(2)}, e^{(3)}, e^{(4)}\}$ or $e(\nabla u) = e^{(5)}$ or $e(\nabla u) = e^{(6)}$ (or $e(\nabla u) \in \{e^{(5)}, e^{(6)}\}$ if $\delta = 0$). Thus, if $\delta \notin \{\pm\frac{3}{2}, \pm 3\}$ it remains to study the 4-well problem $e(\nabla u) \in \{e^{(1)}, e^{(2)}, e^{(3)}, e^{(4)}\}$. Here, the strain equations turn into

$$\begin{aligned}0 &= \partial_1\partial_2e_{12}, \\ 0 &= \partial_1(-\partial_1e_{23} + \partial_2e_{13}), \\ 0 &= \partial_2(\partial_1e_{23} - \partial_2e_{13}).\end{aligned}$$

Remark 32. If $\delta = \pm\frac{3}{2}$ the previous argument does not yield a result which is as strong as the one above. This is due to the fact that in the case $\delta = \pm\frac{3}{2}$ it is possible that up to *five* matrices satisfy the condition $e_{33} = \text{const}$. in the given planes. Hence, in the case $\delta = \pm\frac{3}{2}$, configurations involving five different strains are not excluded by the previous argument (c.f. the appendix).

In the sequel the structure of solutions of the 4-well problem

$$e(\nabla u) \in \{e^{(1)}, e^{(2)}, e^{(3)}, e^{(4)}\}$$

is examined. For that purpose it has to be remarked that the two-dimensionality of the strain $e = e(y_1, y_2)$ does not imply the two-dimensionality of the displacement fields involved. Yet, the following statement holds:

Lemma 25. *Let $U \subset \mathbb{R}^3$ be open, convex. Let $e(\nabla u) \in L^\infty(U, \mathbb{R}_{sym}^{3 \times 3})$, $e(\nabla u) = e(y_1, y_2)$ be a strain tensor corresponding to a displacement field $u : U \rightarrow \mathbb{R}^3$, $u \in W^{1, \infty}(U, \mathbb{R}^3)$ with $e(\nabla u) \in \{e^{(1)}, e^{(2)}, e^{(3)}, e^{(4)}\}$ in U . Then there exists $v \in H_{loc}^1(U)$, such that locally the following dichotomy holds:*

1.

$$e(\nabla u) = \begin{pmatrix} d_1/2d & e_{12}(y_1) & \partial_1 v(y_1, y_2) + Cy_2 \\ e_{12}(y_1) & d_2/2d & \partial_2 v(y_1, y_2) - Cy_1 \\ \partial_1 v(y_1, y_2) + Cy_2 & \partial_2 v(y_1, y_2) - Cy_1 & d_3/2d \end{pmatrix}$$

or

2.

$$e(\nabla u) = \begin{pmatrix} d_1/2d & e_{12}(y_2) & \partial_1 v(y_1, y_2) + Cy_2 \\ e_{12}(y_2) & d_2/2d & \partial_2 v(y_1, y_2) - Cy_1 \\ \partial_1 v(y_1, y_2) + Cy_2 & \partial_2 v(y_1, y_2) - Cy_1 & d_3/2d \end{pmatrix}.$$

Proof of Lemma 25. Making use of convolution, we can assume to deal with smooth functions. Due to the characterization of strain tensors in Lemma 20 and the two-dimensionality of the strains, we obtain the following system of equations

$$\partial_1 \partial_2 e_{12} = 0, \quad (6.6.1)$$

$$\nabla \left(\nabla \times \begin{pmatrix} e_{13} \\ e_{23} \end{pmatrix} \right) = 0. \quad (6.6.2)$$

For the argument we proceed in two steps:

Step 1: *Discrete wave argument.*

Recalling the convexity of the domain and the two-dimensionality of the strains, the structure of the solution of the wave equation (6.6.1) can be determined explicitly:

$$e_{12}(y_1, y_2) = f_{12}(y_1) + g_{12}(y_2).$$

Further the two-valuedness of e_{12} implies that locally only a single wave can be non-constant:

$$e_{12}(y_1, y_2) = f_{12}(y_1) \text{ or } e_{12}(y_1, y_2) = g_{12}(y_2).$$

Step 2: *Curl argument.*

Considering (6.6.2), we immediately obtain

$$\nabla \times \begin{pmatrix} e_{13} \\ e_{23} \end{pmatrix} = 2C$$

for $C \in \mathbb{R}$. Consequently the identity

$$\nabla \times \begin{pmatrix} e_{13} - Cy_2 \\ e_{23} + Cy_1 \end{pmatrix} = 0$$

combined with Poincaré's lemma yields

$$\begin{pmatrix} e_{13} \\ e_{23} \end{pmatrix} = \nabla v + \begin{pmatrix} -Cy_2 \\ Cy_1 \end{pmatrix},$$

with $v \in H_{loc}^1(U)$. □

With the previous lemma the “outer structure” of the martensite configuration is determined. It remains to argue that the “inner structure” is given by the claimed “zig-zag-bands”. For that purpose we reason that the affine rotation field must vanish, i.e. $C = 0$. In the periodic or whole space case this would be no issue, in the case of a domain with finite diameter we make use of an appropriate change of coordinates. In these the zig-zag-structures are straightened out.

Lemma 26. *1. Let $C \in \mathbb{R}$ and $U \subset \mathbb{R}^2$ be an open, convex domain. Assume that $e_{12}, e_{13}, e_{23} : U \rightarrow \{-1, 1\}$ with*

$$e_{13} - e_{12}e_{23} = 0, \tag{6.6.3}$$

$$e_{12} = e_{12}(y_1), \tag{6.6.4}$$

are given. Let $u : U \rightarrow \mathbb{R}$, $u \in W^{1,\infty}(U, \mathbb{R})$ satisfy

$$\nabla u = \begin{pmatrix} e_{13} \\ e_{23} \end{pmatrix} + \begin{pmatrix} -Cy_2 \\ Cy_1 \end{pmatrix}. \tag{6.6.5}$$

Then we have $C = 0$.

2. In particular this implies that in the situation of Lemma 25 we have $C = 0$.

Remark 33. Condition (6.6.3) is essential for the statement to be true: Using convex integration techniques one can show that a similar statement lacking this additional restriction is false.

Proof of Lemma 26. We give the argument for the second statement first: As pointed out in Lemma 25 we have

$$\begin{pmatrix} e_{13} \\ e_{23} \end{pmatrix} = \nabla v + \begin{pmatrix} -Cy_2 \\ Cy_1 \end{pmatrix}.$$

Without loss of generality we can restrict to case (1) of Lemma 25 and thus, $e_{12} = e_{12}(y_1)$. As the structure of the strains implies that (6.6.3) is satisfied, the first statement of the present lemma can be applied.

In order to verify the first statement of the lemma, we multiply (6.6.5) with the

vector $\begin{pmatrix} 1 \\ -e_{12}(y_1) \end{pmatrix}$ to obtain

$$\partial_1 u(y_1, y_2) - e_{12}(y_1) \partial_2 u(y_1, y_2) = -C y_2 - C e_{12}(y_1) y_1. \quad (6.6.6)$$

Taking into account (6.6.4) and defining $E_{12}(y_1)$ via

$$E'_{12}(y_1) = e_{12}(y_1), \quad E_{12}(0) = 0,$$

(6.6.6) can be reformulated as

$$\frac{d}{dy_1}(u(y_1, y_2 - E_{12}(y_1))) = -C y_2 + h(y_1)$$

for a function h . Integrating this, results in

$$u(y_1, y_2 - E_{12}(y_1)) = -C y_1 y_2 + H(y_1) + k(y_2),$$

where k is a generic function of y_2 . Taking the y_2 -derivative yields

$$\partial_2 u(y_1, y_2 - E_{12}(y_1)) = -C y_1 + k'(y_2). \quad (6.6.7)$$

By combining (6.6.5) and (6.6.7), we find

$$\{-1, 1\} \ni e_{23}(y_1, y_2 - E_{12}(y_1)) = -2C y_1 + k'(y_2).$$

Varying y_1 for fixed y_2 yields the desired result, $C = 0$, as otherwise the left hand side of the equation were discrete, while the right hand side were depending on y_1 continuously. \square

Lemma 27. *Let $u : \mathbb{R}^2 \rightarrow \mathbb{R}$, $u \in W^{1,\infty}(\mathbb{R}^2, \mathbb{R})$. Let $\Phi(s, t) : \mathbb{R}^2 \rightarrow \mathbb{R}^2$ be bilipschitz, $\gamma_t(s) := \Phi(s, t)$.*

Then for \mathcal{L}^1 a.e. t we have that for \mathcal{L}^1 a.e. s , the function $(u \circ \gamma_t)(s)$ is classically differentiable and the classical chain rule holds:

$$\frac{d}{ds}(u \circ \gamma_t)(s) = \partial_1 u(\gamma_t(s)) \gamma'_{t1}(s) + \partial_2 u(\gamma_t(s)) \gamma'_{t2}(s). \quad (6.6.8)$$

Proof of Lemma 27. In order to prove the statement of the lemma we have to show that Rademacher's theorem holds for $u \circ \Phi$. For this purpose it suffices to prove that a Lipschitz function maps sets of measure zero to sets of measure zero. Thus, let $N \subset \mathbb{R}^2$ be a null set and $\epsilon > 0$ be arbitrary. Then N can be covered by countably many cubes Q_k with $\sum_{k=1}^{\infty} \mathcal{L}^2(Q_k) < \epsilon$. The Lipschitz property of Φ implies that $\Phi(Q_k \cap N)$ can be covered by cubes of the size $\text{Lip}(\Phi)^2 \mathcal{L}^2(Q_k)$, which yields a bound of $\epsilon \text{Lip}(\Phi)^2$ for the image set $\Phi(N)$. Letting $\epsilon \downarrow 0$ proves the claim. \square

Proposition 27. *Let $U \subset \mathbb{R}^3$ be open, convex. Let $e \in L^\infty(U, \mathbb{R}_{sym}^{3 \times 3})$, $e(\nabla u) = e(y_1, y_2)$ be a strain tensor associated with a displacement field $u : U \rightarrow \mathbb{R}^3$, $u \in W^{1,\infty}(U, \mathbb{R}^3)$, with $e(\nabla u) \in \{e^{(1)}, e^{(2)}, e^{(3)}, e^{(4)}\}$ in U .*

Then in situation (1) of Lemma 25 the configuration of the phases locally corresponds to a crossing twin structure: More precisely, there exists $g \in L^\infty(\mathbb{R}^3)$ such that locally

$$e_{12} = e_{12}(y_1), (e_{13} \circ \Phi)(s, t) = e_{12}(s)g(t), (e_{23} \circ \Phi)(s, t) = g(t),$$

where $\Phi(s, t) = (s, t - E_{12}(s))$ and $E'_{12}(s) = e_{12}(s)$, $E_{12}(0) = 0$.

Due to symmetry reasons similar results also hold for case (2) of Lemma 25.

Proof of Proposition 27. In situation (1) of Lemma 25 the discreteness of the strains gives rise to the following algebraic relation which can – in the notation of Lemma 26 – be reformulated in terms of the function v :

$$\begin{aligned} e_{13}(y_1, y_2) - e_{12}(y_1)e_{23}(y_1, y_2) &= 0 \\ \Rightarrow \partial_1 v(y_1, y_2) - e_{12}(y_1)\partial_2 v(y_1, y_2) &= 0. \end{aligned} \quad (6.6.9)$$

Defining $\gamma_t(s) := (s, t - E_{12}(s))$ and noticing that $\Phi(s, t) := (s, t - E_{12}(s))$ is by definition a bilipschitz mapping with inverse $\Psi(s, t) := (s, t + E_{12}(s))$, Lemma 27 can be applied. Consequently the chain rule yields

$$\frac{d}{ds}(v(\Phi(s, t))) = \partial_1 v(s, t - E_{12}(s)) - e_{12}(s)\partial_2 v(s, t - E_{12}(s)) \stackrel{(6.6.9)}{=} 0.$$

Finally, using the given change of coordinates, we obtain the desired result:

$$\begin{aligned} \begin{pmatrix} e_{13} \circ \Phi \\ e_{23} \circ \Phi \end{pmatrix} &= \begin{pmatrix} (\partial_1 v) \circ \Phi \\ (\partial_2 v) \circ \Phi \end{pmatrix} = \begin{pmatrix} 1 & e_{12}(s) \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \partial_s(v \circ \Phi)(s, t) \\ \partial_t(v \circ \Phi)(s, t) \end{pmatrix} \\ &= \begin{pmatrix} 1 & e_{12}(s) \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ \partial_t v(t) \end{pmatrix} \\ &= \begin{pmatrix} e_{12}(s)\partial_t v(t) \\ \partial_t v(t) \end{pmatrix}. \end{aligned}$$

□

Proof of Proposition 23

Due to the piecewise polygonal structure of the configuration under consideration, we can rely on the classification result of the homogeneous case: Via a “blow-up procedure” at the respective corners we may deduce that any corner or any edge corresponds to one of the homogeneous constructions.

Lemma 28. *Consider a piecewise polygonal configuration determined by its deformation u . Any corner involved in this arrangement of strains corresponds to one of the homogeneous constructions. Any edge corresponds to one of the compatible edges provided by the affine calculations.*

Proof. We consider a “blow-up” of the deformation u at a given corner. Without loss of generality, we may assume that the corner is located at $x = 0$ and the deformation vanishes at that point, $u(0) = 0$. Furthermore, due to the polygonal structure of the strain configuration, we may suppose that the configuration is zero-homogeneous in $B_2(0)$ (else we choose a smaller radius). For $0 < \lambda \ll 1$ we consider the following rescaled version of u :

$$v_\lambda(x) := \frac{u(\lambda x)}{\lambda}.$$

As $u \in W^{1,\infty}$ and $u(0) = 0$, $v_\lambda \xrightarrow{*} v$ in $W_{loc}^{1,\infty}$ for a subsequence $\lambda_k \rightarrow 0$. Moreover,

$$e(\nabla v_\lambda)(x) = e(\nabla u)(\lambda x).$$

Thus, the zero-homogeneity of $e(\nabla u)$ implies the existence of a pointwise limit of $e(\nabla v_\lambda)$ which is independent of the sequence $\lambda \rightarrow 0$ and is zero-homogeneous. Furthermore, the limiting strain corresponds to $e(\nabla v)$ by virtue of the uniqueness of limits. As a consequence, $e(\nabla v)$ has a corner at $x = 0$. This corner coincides with the corner of u at $x = 0$ and it corresponds to one of the classified homogeneous ones. This implies the desired result. \square

Remark 34. • Instead of using a “blow-up procedure”, it would have been possible to argue via Liouville’s theorem.

- The blow-up lemma links the homogeneous case with the piecewise polygonal situation. It can be interpreted as a local classification result. As a consequence, the following analysis can rely on local information in order to obtain a global rigidity result.

Before proving the proposition, we point out the following central observation which is true for $\delta \notin \{\pm\frac{3}{2}, \pm 3\}$.

Observation 2. *All the crossing twin structures are planar. The planes which separate the different phases involved in a corner intersect in a line. We call this line the invariant line of the associated corner. Along this line there cannot be a further jump, as locally the invariant line is surrounded by four different phases. Therefore, if another plane with different phases intersected the invariant line, we would obtain a corner of degree larger than four. This would contradict the characterization of homogeneous corners, as we could carry out a blow-up at this point.*

With this we can come to the proof of the desired result.

Proof of Proposition 23. Step 1: Elimination of boundary effects.

In the sequel, we only deal with the case $\Omega = \mathbb{R}^3$. The case of a general bounded domain can, however, be treated similarly: The slopes of the invariant lines (and of the twinning planes) determine the size of the global constant $c > 0$ from the Proposition. More precisely, it can be chosen such that whenever a configuration in $B_c(0)$ is compatible but not a twin or crossing twin configuration, the non-admissible point must lie in $B_1(0)$. This can be achieved as there are only a finite and fixed number of possible slopes for the jump planes and the invariant lines (compare with the \mathbb{R}^3 argument below).

Step 2. Combinatorics.

We argue via contradiction. If there were a configuration which is neither laminar nor a crossing twin, then there would exist at least one four-fold corner corresponding to one of the above classified homogeneous ones. As we assume that the configuration is not globally given by a crossing twin configuration, there is a plane intersecting the configuration determined by our corner which is not compatible with a crossing twin configuration. As we have excluded boundary effects, this plane has to cross at least two phases of the original four-fold corner (here, we have two possibilities: either the intersection is in a straight line or it is a result of two lines intersecting the two original phases, c.f. Fig. 6.7).

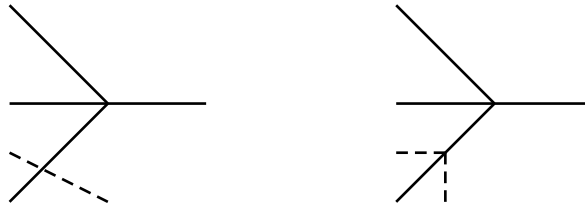


Figure 6.7: Possible intersections. The dashed lines depict the possible intersection implying a change of the original four-fold corner.

Since this causes an at least three-fold corner, the classification of homogeneous corners implies that at this point there is a second four-fold corner. Moreover, the original and the new four-fold corner have a common jump plane (c.f. Fig. 6.8).

Therefore, the respective invariant lines of the two corners are located in this plane. This yields two possible scenarios: Either the invariant lines are parallel or they are not. As the invariant lines are located in the same plane the second case implies that the lines have an intersection point. By our observations on invariant lines this leads to a contradiction. Thus, the remaining alternative consists of the invariant lines being parallel.

In this case we are left with globally planar configurations (if the configuration were not globally planar we could repeat the argument from above). Reviewing all

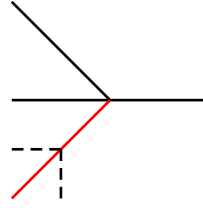


Figure 6.8: Common intersection plane of four-fold corners. The dashed lines depict the new four-fold corner. It shares a jump plane with the original four-fold corner.

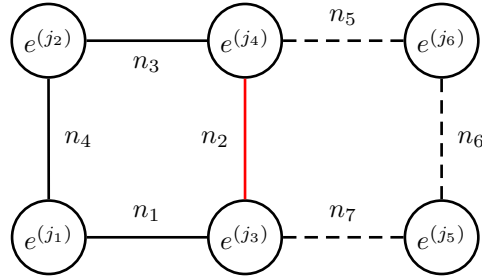


Figure 6.9: Arrangement of planar phases. The schematic picture illustrates that the neighbouring corners share at least a common jump plane and have two strain variants in common.

homogeneous constructions (c.f. Fig. 6.4, 6.5, 6.6) and taking into account that the respective corners have to share two strain variants along a common normal, we note that all possible planar situations are given by the following normal vectors and strains:

$$\begin{aligned}
 & [1, 0, 0], [0, 1, 1], [0, 1, -1] \text{ together with the strains } e^{(1)}, e^{(2)}, e^{(3)}, e^{(4)}, \\
 & [0, 1, 0], [1, 0, 1], [1, 0, -1] \text{ together with the strains } e^{(1)}, e^{(2)}, e^{(5)}, e^{(6)}, \\
 & [0, 0, 1], [1, 1, 0], [1, -1, 0] \text{ together with the strains } e^{(3)}, e^{(4)}, e^{(5)}, e^{(6)}.
 \end{aligned}$$

Hence, it suffices to consider strain configurations which globally only depend on the variables normal to one of these vectors. Due to the results of the section on planar strains, Section 6.6, these configurations are either given by laminates or by crossing twin structures. This proves the proposition. \square

6.7 Appendix

A Combinatorial Proof of Lemma 24 and Proposition 25 in the Case $\delta \notin \{\pm\frac{3}{2}, \pm 3\}$

As an alternative to a Mathematica aided proof, the arguments leading to Lemma 24 and Proposition 25 can also be carried out “by hand”. In order to do so, we follow the same strategy as in the computer aided situation:

- As an initial step, we identify points on the sphere which lie at the intersection

of the possible jump planes. We notice that there are at most corners of degree eight. Thus, in a first step, we focus on the points involving three or more possible jump planes, in other words, on the points of possible maximal degree six or eight.

- Secondly, we argue that at these points of potentially high order the local configurations can at most consist of crossing twins. Furthermore, we show that these can only occur at very specific points. In particular, at many of the determined possible high order intersection points only laminates can form.
- Finally, we prove that at the remaining intersection points, i.e. at those of maximal degree four, which were not treated as parts of the higher order cases, only laminates can be observed.

We recall that the normals of the possible jump planes associated with the cubic-to-orthorhombic phase transition are given by

$$\begin{aligned} & \{[1, 0, 0], [0, 1, 1], [0, 1, -1], [0, 1, 0], [1, 0, 1], [1, 0, -1], [0, 0, 1], [1, 1, 0], \\ & [1, -1, 0], [3, 3, 2\delta], [3, 2\delta, 3], [2\delta, 3, 3], [3, 3, -2\delta], [3, -2\delta, 3], [-2\delta, 3, 3], \\ & [-2\delta, -3, 3], [-2\delta, 3, -3], [-3, -2\delta, 3], [3, -2\delta, -3], [-3, 3, -2\delta], \\ & [3, -3, -2\delta]\}. \end{aligned} \quad (6.7.1)$$

We note that the sign of the normals is irrelevant. From these we compute all points of intersection on the sphere in which three or more planes meet. As a first observation, we note that for any $\delta \neq \pm 3$ at most four different planes intersect in one point (this can be seen by checking how many different planes have normals lying in a common given plane). Starting from this, we list all the intersection points involving three or four planes.

If $\delta \notin \{\pm\frac{3}{2}, \pm 3\}$ then there are nine possible eight fold corners (i.e. corners involving four planes) at the points $(1, 0, -1)$, $(1, 0, 1)$, $(0, 1, 0)$ (as well as the corresponding permutations of the entries). Up to the corresponding (three) permutations each, these are given by the planes with the following normals:

$$\begin{array}{lll} [1, & 0, & 1] & [-1, & 0, & 1] & [& 1, & 0, & 1] \\ [0, & 1, & 0] & [& 0, & 1, & 0] & [-1, & 0, & 1] \\ [3, & 2\delta, & 3] & [-3, & 2\delta, & 3] & [& 1, & 0, & 0] \\ [3, & -2\delta, & 3] & [-3, & -2\delta, & 3] & [& 0, & 0, & 1]. \end{array}$$

(In the first and second configurations, one can think of the respective permutations as being determined by moving the δ entries to the first, second and third position – and shifting the entries of the other normals correspondingly. In the third configuration the position of the zero in the $[1, 0, 1]$ and $[-1, 0, 1]$ normals yields the different possibilities.)

As these configurations are, by definition, two-dimensional and as their respective normals are given by (a permutation of) one of the vectors $[1, 0, -1]$, $[1, 0, 1]$, $[0, 1, 0]$, the result on planar configurations with these normals, Proposition 26, implies that at any such corner there can at most be crossing twins.

Apart from the corners involving four normals, there are also corners involving three normals. For a generic δ , i.e. $\delta \notin \{\pm\frac{3}{2}, \pm 3\}$, there are the following possibilities $(a_1) - (c)$:

$$\begin{array}{ll}
 (a_1) & (a_2) \\
 [1, 0, 0] & [1, 0, 0] \\
 [3, 2\delta, \pm 3] & [3, \pm 3, 2\delta] \\
 [-3, 2\delta, \pm 3] & [-3, \pm 3, 2\delta],
 \end{array}$$

with corresponding intersection points $(0, \mp 3, 2\delta)$ and $(0, 2\delta, \mp 3)$. Cases (a_1) and (a_2) are symmetry related via a rotation of 90° in the x_2, x_3 plane. Considering all possible permutations, these correspond to a total of 12 possibilities.

Further cases are given by

$$\begin{array}{llll}
 (b_1) & (b_2) & (b_3) & (b_4) \\
 [1, -1, 0] & [1, -1, 0] & [1, 1, 0] & [1, 1, 0] \\
 [2\delta, 3, \pm 3] & [-2\delta, 3, \pm 3] & [3, -2\delta, \pm 3] & [2\delta, 3, \pm 3] \\
 [3, 2\delta, \pm 3] & [3, -2\delta, \pm 3] & [-2\delta, 3, \mp 3] & [3, 2\delta, \mp 3],
 \end{array}$$

with corresponding intersection points given by $(1, 1, \mp(1 + \frac{2\delta}{3}))$, $(1, 1, \mp(1 - \frac{2\delta}{3}))$, $(1, -1, \mp(1 + \frac{2\delta}{3}))$, $(-1, 1, \mp(1 - \frac{2\delta}{3}))$. We remark that $(b_3), (b_4)$ are rotations by 90° of $(b_1), (b_2)$. Considering all possible permutations, cases $(b_1) - (b_4)$ correspond to a total of 24 possibilities.

Finally, the only remaining corners involving three normals are given by

$$\begin{array}{llll}
 & [0, 1, -1] & [0, 1, 1] & [0, 1, 1] & [0, 1, -1] \\
 (c) & [1, 0, -1] & [1, 0, 1] & [-1, 0, 1] & [1, 0, 1] \\
 & [1, -1, 0] & [-1, 1, 0] & [1, 1, 0] & [1, 1, 0],
 \end{array}$$

with the intersection points $(1, 1, 1), (1, 1, -1), (1, -1, 1), (-1, 1, 1)$. (That there are no further corners at which three planes intersect, can, for example, be seen by computing the determinants of all the remaining three tuples of normals. In the cases $\delta \notin \{\pm\frac{3}{2}, \pm 3\}$ these are nontrivial.)

Combining the previous considerations, we obtain that in the generic case there are

$$\begin{aligned}
& \#(\text{number of possible four-fold corners}) \\
& - \#(\text{number of possible six-fold corners}) \left(\binom{3}{2} - 1 \right) \\
& - \#(\text{number of possible eight-fold corners}) \left(\binom{4}{2} - 1 \right) \\
& = 210 - 40 \times 2 - 9 \times 5 = 85
\end{aligned}$$

intersection points at which the possible configurations have to be investigated. As we will see from Observation 3, symmetry considerations reduce the previously described configurations (a₁) – (c) to only *three* (instead of 10) different cases.

In order to understand that only crossing twins and laminates can appear, we have to exclude other possible configurations emerging from the corners with possibly three intersecting planes. By symmetry considerations it will be possible to reduce the situation to the following two auxiliary results:

Proposition 28. *Let $e = e(\nabla u) = \frac{1}{2}(\nabla u + (\nabla u)^t)$, with $u : \Omega \rightarrow \mathbb{R}^3$ Lipschitz. Assume that $e \in \{e^{(i_1)}, e^{(i_2)}, e^{(i_3)}\}$ with*

$$e^{(i_1)} \in \{e^{(1)}, e^{(2)}\}, \quad e^{(i_2)} \in \{e^{(3)}, e^{(4)}\}, \quad e^{(i_3)} \in \{e^{(5)}, e^{(6)}\}. \quad (6.7.2)$$

Suppose that $\delta \notin \{\pm\frac{3}{2}, \pm 3\}$. Then, locally, e is a simple laminate.

Proof. The proposition follows from the fact that if a three valued strain satisfies (6.7.2), then it can be mapped to the corresponding Dolzmann-Müller situation, Proposition 24. In order to prove this, we notice that (with the normalization of (6.7.1)) the rank-one connections between the strains $e^{(i_1)}, e^{(i_2)}, e^{(i_3)}$ each involve a normal with and a normal without δ entries. Denoting the normals with δ entries by n_i^δ , a mapping to the Dolzmann-Müller case is given by

$$(M^\delta)^{-1} : (n_1^\delta, n_2^\delta, n_3^\delta) \mapsto (n_1^0, n_2^0, n_3^0),$$

which sends the normals involving δ entries to the ones with $\delta = 0$. In order to check that this indeed fulfills the desired mapping properties, it suffices to carry out the computations for the three-tuples satisfying

$$\begin{aligned}
(e^{(i_1)}, e^{(i_2)}, e^{(i_3)}) \in \{ & (e^{(1)}, e^{(3)}, e^{(5)}), (e^{(1)}, e^{(4)}, e^{(5)}), (e^{(1)}, e^{(4)}, e^{(6)}), \\
& (e^{(1)}, e^{(3)}, e^{(6)}) \},
\end{aligned}$$

since the remaining cases follow by reflecting δ : $\delta \mapsto -\delta$. As an example, we carry out one of these computations: In case of $(e^{(1)}, e^{(3)}, e^{(5)})$ such a mapping would for

example be given by

$$\begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix} \mapsto \begin{pmatrix} 2\delta \\ 3 \\ -3 \end{pmatrix}, \quad \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} \mapsto \begin{pmatrix} 3 \\ -3 \\ -2\delta \end{pmatrix}, \quad \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \mapsto \begin{pmatrix} 3 \\ 2\delta \\ 3 \end{pmatrix},$$

or

$$M := M^\delta = \frac{1}{2} \begin{pmatrix} 6 + 2\delta & 2\delta & -2\delta \\ 2\delta & 6 + 2\delta & 2\delta \\ -2\delta & 2\delta & 6 + 2\delta \end{pmatrix}.$$

Then the strains, $\hat{e}^{(i)} = M^{-1}e^{(i)}M^{-t}$, in the new coordinates turn into

$$\begin{aligned} \hat{e}^{(1)} &= \begin{pmatrix} \frac{9-7\delta^2}{4(-3+\delta)^2(3+2\delta)^2} & \frac{\delta(3+\delta(2+\delta))}{4(-3+\delta)^2(3+2\delta)^2} & -\frac{\delta(3+\delta(2+\delta))}{4(-3+\delta)^2(3+2\delta)^2} \\ \frac{\delta(3+\delta(2+\delta))}{4(-3+\delta)^2(3+2\delta)^2} & \frac{9-7\delta^2}{4(-3+\delta)^2(3+2\delta)^2} & \frac{\delta(3+\delta(2+\delta))}{4(-3+\delta)^2(3+2\delta)^2} \\ -\frac{\delta(3+\delta(2+\delta))}{4(-3+\delta)^2(3+2\delta)^2} & \frac{\delta(3+\delta(2+\delta))}{4(-3+\delta)^2(3+2\delta)^2} & \frac{-9+\delta^2-\delta^3}{2(-3+\delta)^2(3+2\delta)^2} \end{pmatrix}, \\ \hat{e}^{(3)} &= \begin{pmatrix} \frac{9-7\delta^2}{4(-3+\delta)^2(3+2\delta)^2} & \frac{\delta(3+\delta(2+\delta))}{4(-3+\delta)^2(3+2\delta)^2} & -\frac{\delta(3+\delta(2+\delta))}{4(-3+\delta)^2(3+2\delta)^2} \\ \frac{\delta(3+\delta(2+\delta))}{4(-3+\delta)^2(3+2\delta)^2} & \frac{-9+\delta^2-\delta^3}{2(-3+\delta)^2(3+2\delta)^2} & \frac{\delta(3+\delta(2+\delta))}{4(-3+\delta)^2(3+2\delta)^2} \\ -\frac{\delta(3+\delta(2+\delta))}{4(-3+\delta)^2(3+2\delta)^2} & \frac{\delta(3+\delta(2+\delta))}{4(-3+\delta)^2(3+2\delta)^2} & \frac{9-7\delta^2}{4(-3+\delta)^2(3+2\delta)^2} \end{pmatrix}, \\ \hat{e}^{(5)} &= \begin{pmatrix} \frac{-9+\delta^2-\delta^3}{2(-3+\delta)^2(3+2\delta)^2} & \frac{\delta(3+\delta(2+\delta))}{4(-3+\delta)^2(3+2\delta)^2} & -\frac{\delta(3+\delta(2+\delta))}{4(-3+\delta)^2(3+2\delta)^2} \\ \frac{\delta(3+\delta(2+\delta))}{4(-3+\delta)^2(3+2\delta)^2} & \frac{9-7\delta^2}{4(-3+\delta)^2(3+2\delta)^2} & \frac{\delta(3+\delta(2+\delta))}{4(-3+\delta)^2(3+2\delta)^2} \\ -\frac{\delta(3+\delta(2+\delta))}{4(-3+\delta)^2(3+2\delta)^2} & \frac{\delta(3+\delta(2+\delta))}{4(-3+\delta)^2(3+2\delta)^2} & \frac{9-7\delta^2}{4(-3+\delta)^2(3+2\delta)^2} \end{pmatrix}. \end{aligned}$$

Subtracting a constant matrix given by the off-diagonal entries and renormalizing yields the Dolzmann-Müller situation. \square

We remark that these transformation matrices degenerate in the cases $\delta \in \{\pm\frac{3}{2}, \pm 3\}$.

Lemma 29. *Let $e \in \{e^{(1)}, e^{(2)}, e^{(5)}\}$ be independent of the variable $3x_2 - 2\delta x_3$. Then the only possible homogeneous corners consist of two strain variants, i.e there is a single flat interface and at most two strains are involved. An analogous statement holds for the case $e \in \{e^{(1)}, e^{(2)}, e^{(6)}\}$.*

Proof. We only consider the first case. In this very specific situation we have four linear conditions:

$$\text{tr}(e) = 0, \quad e_{22} = 1, \quad e_{13} = 0, \quad e_{23} = -\frac{\delta}{3}e_{11} + \frac{\delta}{3}.$$

Furthermore, $e = e(x_1, 2\delta x_2 + 3x_3)$. Then the first three strain equations, (6.3.2), yield

$$(-\partial_{11} + \partial_{33})e_{11} = 0,$$

which, due to the two valuedness of the e_{11} component, leads to

$$e_{11} = f(3x_1 + 2\delta x_2 + 3x_3) \text{ or } e_{11} = g(3x_1 - 2\delta x_2 - 3x_3).$$

Considering only the first case, $e_{11} = f(3x_1 + 2\delta x_2 + 3x_3)$, (the argument for the second one is analogous), the remaining three (curl type) strain equations, (6.3.3), yield

$$\begin{aligned} \partial_3(-2\delta\partial_1 + 3\partial_2)e_{12} &= 0, \\ \partial_3(\partial_1 - \partial_3)e_{12} &= 0, \\ \partial_3(-2\delta\partial_1 - 3\partial_2)e_{12} &= 0, \end{aligned}$$

if the expression for e_{11} and the linear dependence of e_{11} and e_{22} is inserted. Due to the assumed structure of e , the transversality of the vectors $[3, 2\delta, 3]$ and $[1, 0, 0]$ and $e_{12} = e_{12}(e_{11})$, this leads to

$$e_{12} = e_{12}(3x_1 + 2\delta x_2 + 3x_3) \text{ or } e_{12} = e_{12}(x_1).$$

Thus, either $e_{11} = \text{const.}$ or if $e_{11} = f(3x_1 + 2\delta x_2 + 3x_3) \neq \text{const.}$ then $e_{12} = e_{12}(3x_1 + 2\delta x_2 + 3x_3)$. In both cases we deduce that the configuration is a simple laminate. \square

Last but not least, we have to show that any corner involving three normals satisfies the conditions of Proposition 28 or of Lemma 29. Furthermore, we have to identify those intersection points at which crossing twin structures can appear. For that purpose, we prove the following claim.

Claim 2. *All corners at which three or four planes intersect and which are not located at (up to permutations) one of the points $(1, 0, 0)$, $(0, 1, 1)$, $(0, 1, -1)$ involve configurations with at most three strains $e^{(i_1)}, e^{(i_2)}, e^{(i_3)}$. Up to symmetries these satisfy the conditions of Proposition 28 or of Lemma 29.*

This claim then proves Lemma 24, since in the case of three involved strains, Proposition 28 or Lemma 29 assert that the configuration only consists of simple laminates. If only two strains are involved in a possible corner and do not satisfy condition (6.7.2) (restricted to two strains), these strains commute. The strains being simultaneously diagonalizable, implies that these can also be transformed into the Dolzmann-Müller situation. Hence, in that case only simple laminates can occur.

For abbreviation, we use the following convention:

Definition 11. *We use the notation $(2, 3)$ to denote a possible jump between $e^{(2)}$ and $e^{(3)}$.*

Proof of the claim. In order to reduce the situation to as few examples as possible, we make use of the symmetries of the phase transition. We observe

Observation 3. *Any rotation of 90° around one of the coordinate axes transforms compatible corners into compatible corners.*

Under the reflection which leaves the x_1, x_2 -plane invariant, the phases transform according to

$$\begin{array}{lll} e^{(1)} \mapsto e^{(1)}, & e^{(3)} \mapsto e^{(4)}, & e^{(5)} \mapsto e^{(5)}, \\ e^{(2)} \mapsto e^{(2)}, & e^{(4)} \mapsto e^{(3)}, & e^{(6)} \mapsto e^{(6)}. \end{array}$$

Similar results hold for reflections with respect to the other coordinate axes. In particular, reflections with respect to the coordinate axes preserve the assumptions of Proposition 28.

In order to prove the claim, we first rule out more complicated behaviour for the corners involving three normals. We only have to consider the cases (a_1) , (b_1) and (c) , as the other ones follow from symmetry. Note that normals involving δ entries uniquely (up to symmetry) describe a single jump, e.g. at the normal $[2\delta, 3, 3]$ there can only be the jump $(1, 3)$, while the ones without δ entries allow for two possible jumps (up to symmetry), e.g. the normal $[1, 0, 0]$ allows for the jumps $(1, 2)$ and $(3, 4)$. In the sequel, we discuss the cases (a_1) , (b_1) , (c) separately:

- (a_1) We first consider the case of the plus signs. At each of the normals we have the following jump possibilities (here the left column contains the jump normals and the right hand side the possible corresponding jumps associated with the respective normal)

$$\begin{array}{ll} [1, 0, 0] & (1, 2), (3, 4), \\ [3, 2\delta, 3] & (1, 5), \\ [-3, 2\delta, 3] & (2, 5). \end{array}$$

Thus, at this intersection point only the combination of phases $\{e^{(1)}, e^{(2)}, e^{(5)}\}$ or of $\{e^{(3)}, e^{(4)}\}$ is possible. While the second case directly implies that only laminates can appear, we have to invoke Lemma 29 for the first one. By carrying out a reflection with respect to the x_1, x_2 -plane, it is possible to transform the case with the plus signs into that with the minus signs. By Observation 3 this reduces the case of the minus signs to the second case treated in Lemma 29.

- (b_1) We begin with the case with the plus signs. The possibly present phases are given by

$$\begin{array}{ll} [1, -1, 0] & (3, 5), (4, 6), \\ [2\delta, 3, 3] & (1, 3), \\ [3, 2\delta, 3] & (1, 5) \end{array}$$

This corresponds to a three-fold combination $\{e^{(1)}, e^{(3)}, e^{(5)}\}$ and a two-fold

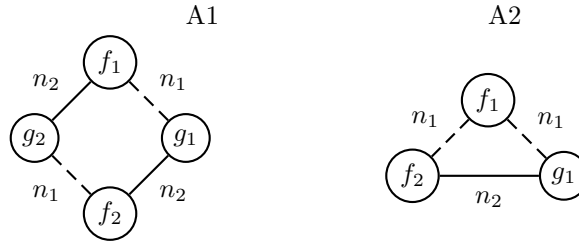


Figure 6.10: Excluding configurations with possible maximal degree four.

combination $\{e^{(4)}, e^{(6)}\}$. In particular, the configuration satisfies the assumptions of Proposition 28. As the case with the minus signs is obtained by a reflection along the x_1, x_2 -plane, Observation 3 asserts that again the conditions of Proposition 28 are fulfilled.

- (c) Due to 180° rotation symmetries (around the coordinate axes), it suffices to consider the first case. Here, the possible normals and jumps are given by:

$$\begin{array}{lll}
 [0, 1, -1] & (1, 3), & (2, 4), \\
 [1, 0, -1] & (1, 5), & (2, 6), \\
 [1, -1, 0] & (3, 5), & (4, 6).
 \end{array}$$

Thus, the admissible configurations involve either only the strains $\{e^{(1)}, e^{(3)}, e^{(5)}\}$ or $\{e^{(2)}, e^{(4)}, e^{(6)}\}$ (which satisfy the requirements of Proposition 28).

Hence, it remains to discuss the corners at which only two planes intersect. Here we have to distinguish three cases:

- *Both normals are elements of $\{[1, 0, 0], [0, 1, 1], [0, 1, -1]\}$ or they are permutations thereof.* In this case the configurations already appeared in the discussion of corners at which three or four planes intersect.
- *Both normals involve δ entries.* Then, at each of the two normals there is a unique jump possibility: (f_1, g_1) and (f_2, g_2) . We claim that in this case only two different strains can be involved in a possible corner. Indeed, the possible configurations are depicted in Figure 6.10. As only two different normals are involved, configurations A1 and A2 schematically illustrate the only possible higher order corners. Since the jumps are uniquely determined by the normals, this implies that the sets $\{f_1, f_2\}$ and $\{g_1, g_2\}$ have to coincide in configuration A1. Due to the same reason, the jumps (f_2, g_1) and (f_1, f_2) have to agree (up to permutations) in configuration A2. This entails that only two phases are involved in the respective configuration. Hence, only simple laminates can occur.
- *Only one of the normals involves δ entries.* This implies that at most three

phases are part of the respective corner as the jumps at the normal involving δ entries are unique. Arguing in the setting of Figure 6.10, one notices that configuration A1 can only consist of two different strains due to the uniqueness of the jump given by the normal involving δ entries. Hence, it remains to investigate the situation of configuration A2. If the normal n_1 corresponds to the normal without δ entries, it would, in principle, be possible that three phases are involved in configuration A2. However, recalling the rank-one connections of the cubic-to-orthorhombic phase transition, we note that the non-uniqueness emerging in jumps involving normals with non- δ -entries is “strictly disjoint”: In other words, if (f_1, g_1) and (f_2, g_2) denote the possible jumps at normals with a non-unique jump, these sets are strictly disjoint – their union involves a total of four different strains. In effect, the situation of configuration A2 can also be excluded. As above, only corners involving two strains emerge. These configurations, however, correspond to simple laminates.

□

The Cases $\delta = \pm\frac{3}{2}$

In this section we briefly comment on the situation of $\delta = \frac{3}{2}$. By symmetry, the case $\delta = -\frac{3}{2}$ can be treated analogously.

The exceptional role of this case is already indicated by the fact that for $\delta = \frac{3}{2}$ various of the normals involving δ entries “collapse”. If $\delta = \frac{3}{2}$ the local situation on the sphere is already highly nontrivial. Apart from the crossing twin structures, there are corners involving three, five, six and seven (not necessarily different) phases (c.f. discussion in Remark 31). For completeness we briefly list the possible configurations at the points $(1, 0, 0)$, $(-\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}})$, $(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}})$. All the other nontrivial intersection points are symmetry related to these. As a consequence, the configurations at the other points can be computed from the ones listed below.

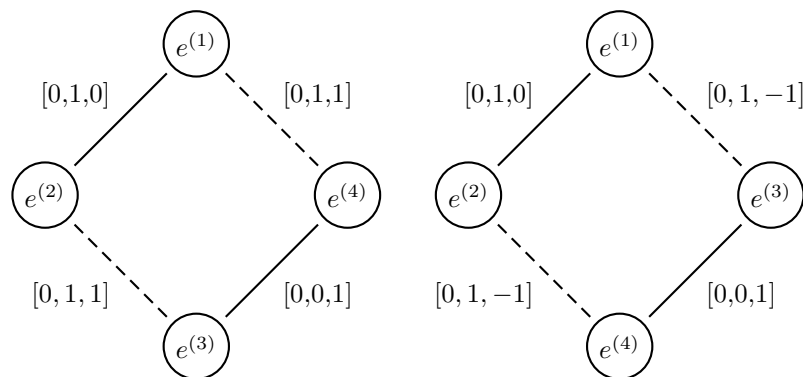


Figure 6.11: Compatible corners at the point $(1, 0, 0)$.

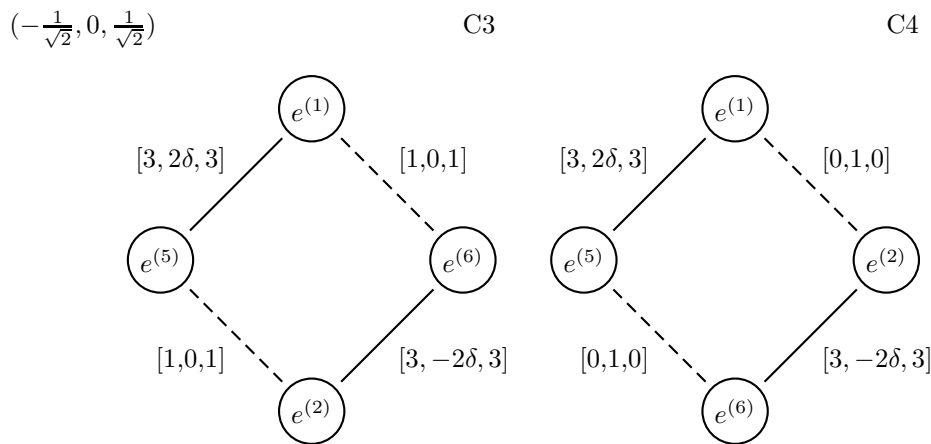


Figure 6.12: Compatible crossing twin configurations at the point $(-\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}})$.

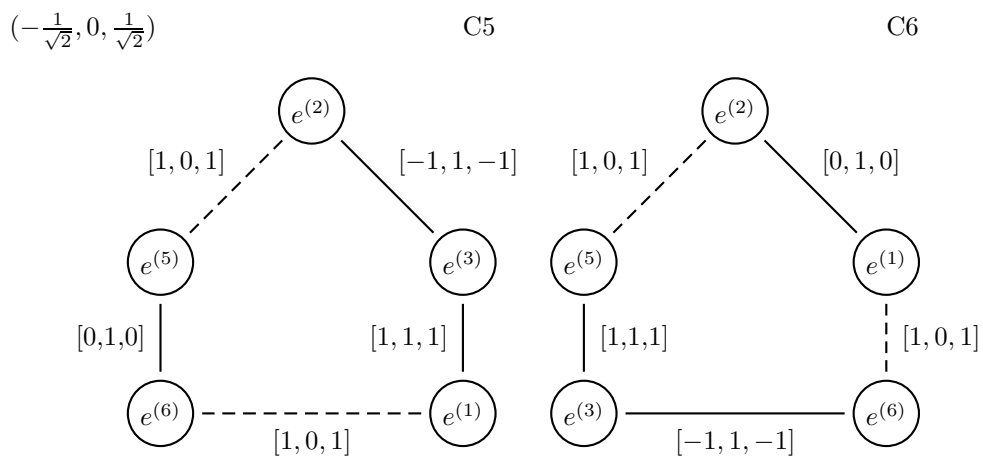


Figure 6.13: Compatible crossing configurations involving five strains at the point $(-\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}})$.

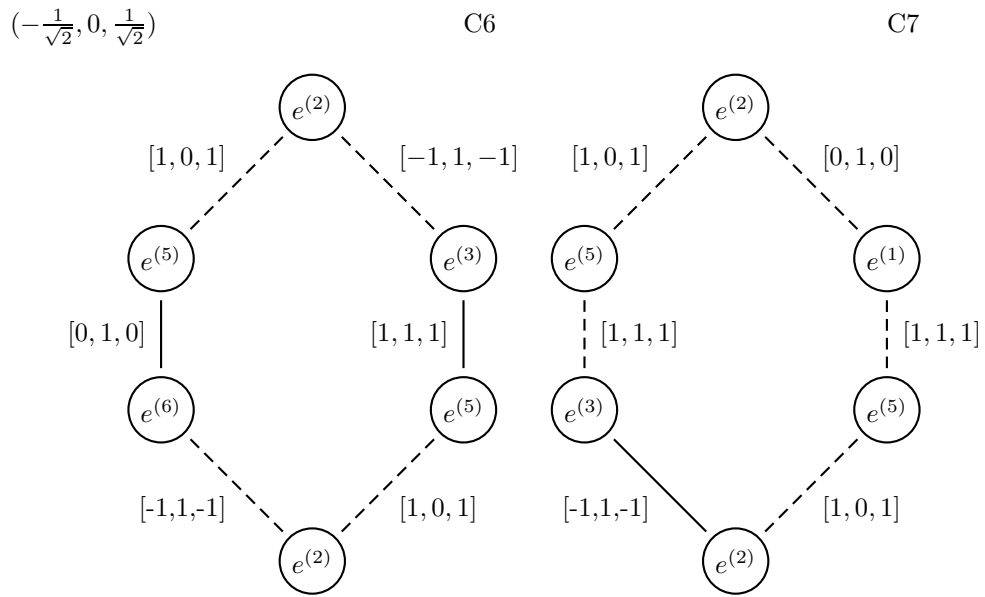


Figure 6.14: Compatible corners involving six strains at the point $(-\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}})$.

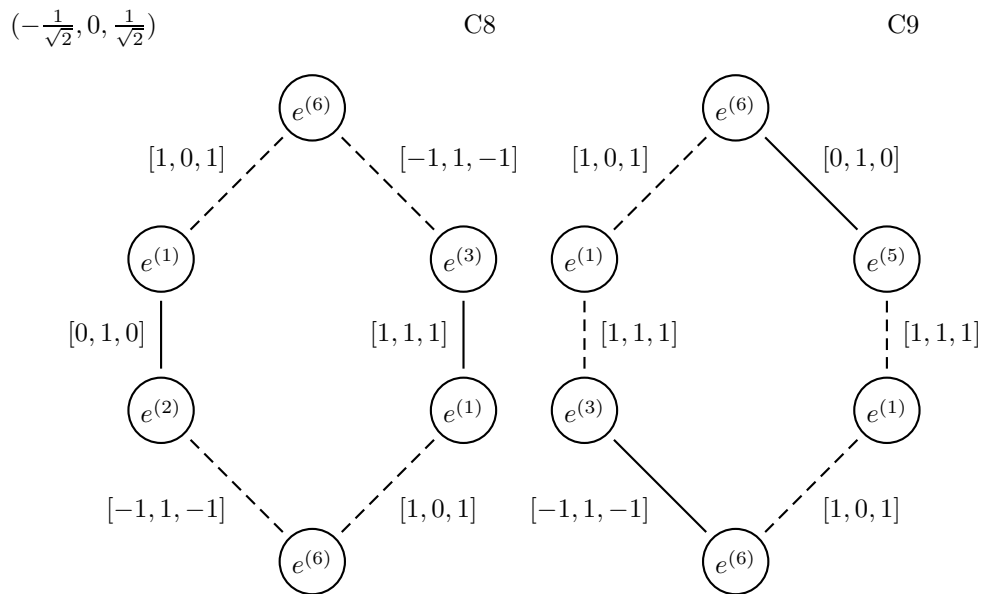


Figure 6.15: Compatible corners involving six strains at the point $(-\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}})$.

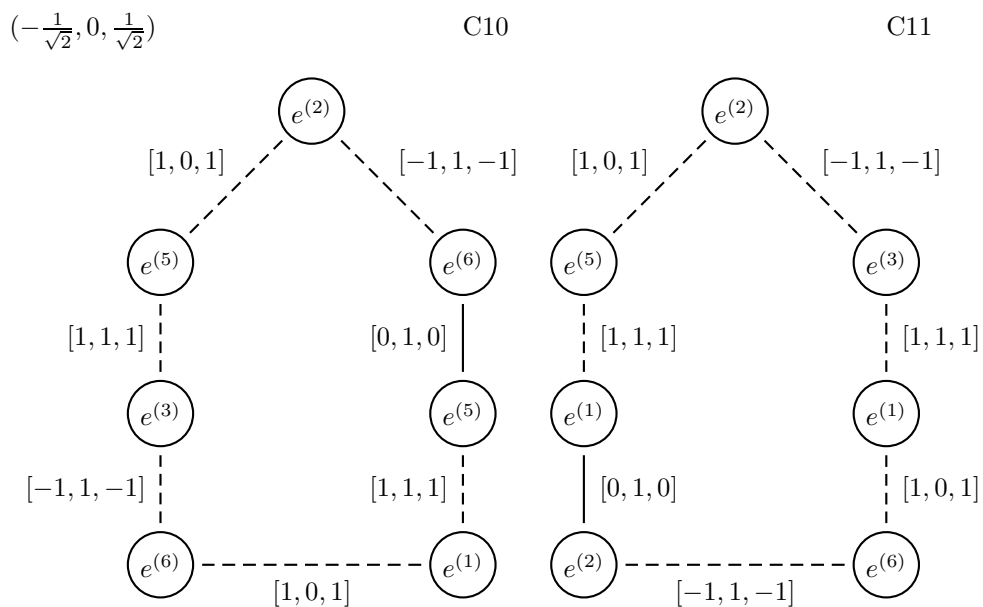


Figure 6.16: Compatible corners involving seven strains at the point $(-\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}})$.

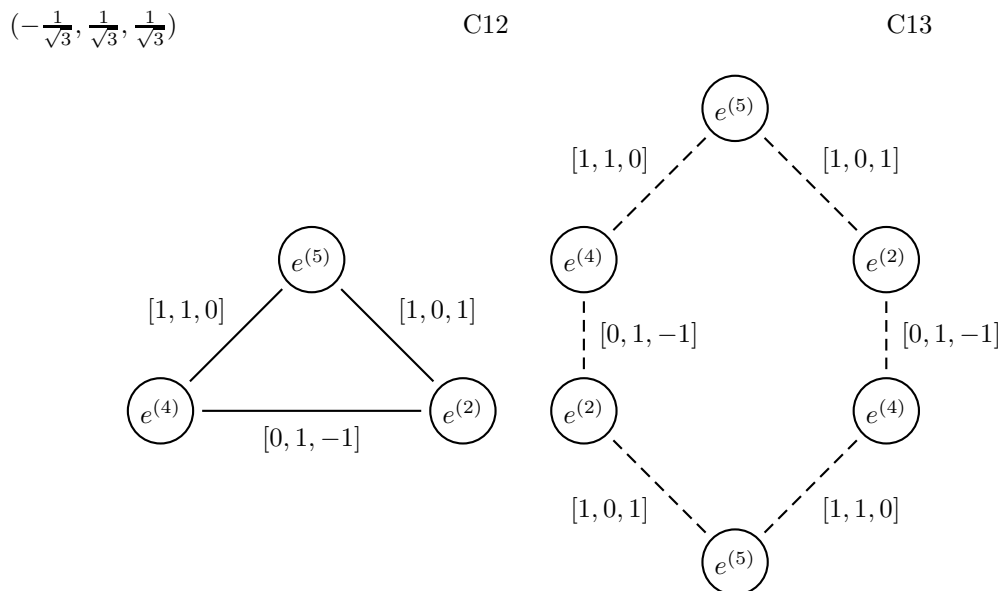


Figure 6.17: Compatible corners involving three and six strains at the point $(-\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}})$.

The Cases $\delta = \pm 3$

We only discuss this situation very briefly. The situation for $\delta = \pm 3$ differs from the generic one by allowing for intersection points involving up to six normals at permutations of the points $(\pm \frac{1}{\sqrt{3}}, \pm \frac{1}{\sqrt{3}}, \pm \frac{1}{\sqrt{3}})$. As a Mathematica based computation illustrates, these intersection points of higher order in fact produce new planar configurations: Even twelve-fold corners can be realized. Due to the large number of possible planar configurations, it is not clear whether they can be combined to yield non-planar global configurations. This would be an interesting topic for future research.

Summary of the Dissertation

In this dissertation, we deal with various rigidity properties in PDEs. We address

- the backward uniqueness problem for the heat equation in conical domains with large opening angles,
- unique continuation for the fractional Laplacian,
- the rigidity and non-rigidity of the so-called cubic-to-orthorhombic phase transition.

These rigidity properties are qualitatively quite different: While the first two problems aim at “extending” the “identity principle” of analytic functions to rougher classes of equations, the third question treats characteristic patterns occurring in certain models of shape-memory alloys. Mathematically, the third problem exhibits properties of hyperbolic equations, while the first two problems display “elliptic and parabolic properties”.

The first two problems deal with the questions of whether a certain vanishing behaviour, i.e.

- vanishing at the final time, in the case of the heat equation in conical domains with large opening angles,
- and vanishing of infinite order at a certain point, in the case of the fractional Laplacian,

implies that the solution of the respective PDE already vanishes globally. In studying these phenomena, we are confronted with possible oscillatory behaviour of solutions of the respective PDE. Thus, the key ingredient of deducing the desired properties consists of proving *highly concentrated, lower* bounds for the respective operators – so-called Carleman inequalities. Establishing such estimates, we prove the backward uniqueness property for the heat equation (with lower order perturbations) in two-dimensional conical domains with opening angles down to approximately 95° . For the fractional Laplacian, we show the unique continuation property involving scaling-critical potentials (with rough lower order perturbations).

In the second part of the thesis, we turn to the so-called cubic-to-orthorhombic phase transition in the theory of shape-memory alloys. Motivated by experimental results in which one observes so-called crossing twin constructions, we aim at a classification of all possible stress-free states. In this context, we prove two complementary results: Using convex integration methods, we show that there is a large number of weak ($W^{1,p}$, $p \in (1, \infty)$) solutions. Complementary to this, we prove that under surface energy constraints (we consider “piecewise polygonal” solutions), this behaviour can be excluded and, locally, only solutions with fixed characteristics, i.e. crossing twin and twin configurations, can emerge.

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PUBLICATIONS	<ul style="list-style-type: none">• Angkana Rüland, <i>The Cubic-to-Orthorhombic Phase Transition: Rigidity and Non-Rigidity</i>, MIS MPI Preprint, 43/2013.• Angkana Rüland, <i>A Rigidity Result for a Reduced Model of a Cubic-to-Orthorhombic Phase Transition in the Geometrically Linear Theory of Elasticity</i>, ArXiv:1305:6200• Angkana Rüland, <i>On the Backward Uniqueness of the Heat Equation in Two-Dimensional Conical Domains</i>, ArXiv:1310.6655, submitted,• Angkana Rüland, <i>Unique Continuation for the Fractional Laplacian with Rough Potentials</i>, in preparation.	
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