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The sharp-interface limit of the Cahn-Hilliard system with elasticity

vorgelegt von

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Introduction

In many different areas we make use of metallic alloys. Turbines are coated with a special Ni-Al alloy and solders made of a Zn-Pl alloy are used to assemble electronic components. These are prominent examples where they serve specific needs, as a turbine should be strengthened and protected to last even in rough environments or chips should have a sufficiently strong mechanical and electrical connection with the board. Here we restrict our analysis to binary alloys, that are alloys based on two materials. We assume that the density is always fixed, so that the concentrations of the respective materials ρ_1 and ρ_2 have to fulfil

$$\rho_1 + \rho_2 = 1$$

everywhere. But then the concentration difference $\rho := \rho_1 - \rho_2$ is sufficient to describe the material distribution:

$$\text{Wherever } \begin{Bmatrix} \rho \sim +1 \\ \rho \sim -1 \end{Bmatrix} \text{ it means that } \begin{Bmatrix} \text{material 1} \\ \text{material 2} \end{Bmatrix} \text{ is dominant.}$$

One problem which often arises is that the homogeneously mixed state, as they are composed to be in, is not stable at normal room temperature. This means that these alloys tend to separate over time, they reverse the mixing and return to a coarse mixture of the original materials. Alloys are usually manufactured at high temperatures. At these high temperatures the homogeneously mixed state is stable – in the thermodynamical language this is described by a free energy function which is convex and has one single minimum, the mixed state. The above-mentioned problem arises when the alloy sample is cooled down to room temperature (here we assume for the simplicity of our model that this happens through a sudden quench to avoid the intermediary cooling effects). At this point, the mixed state becomes instable – this is expressed by a non-convex free energy function which has two distinct minima in $+1$ and -1, see Figure 1. These minima represent the two original materials corresponding to the above remark on the concentration difference.

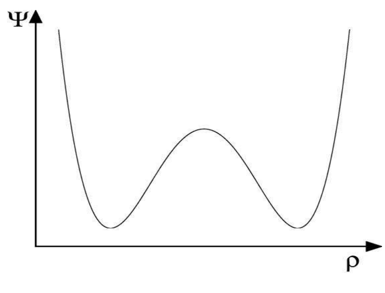

Figure 1: The non-convex free energy function as a double-well potential

The first stage of separation, the so-called spinodal decomposition, happens on a very short time and very small spatial scale: Very quickly a fine micro-structure of many regions consisting of the original materials arises. The concentration difference function has high oscillations between the values $+1$ and -1. Apparently the system tries to minimise the free energy in this first stage.

In the next stage which is called phase re-arrangement we can observe that one material starts to form so-called particles, that is regions or domains, within a so-called matrix by the other material.

Then the coarsening process, also known as Ostwald ripening, takes place. The interfacial area reduces by the growth of the larger particles while smaller particles shrink, see Figures 2 and 3. This has been quantised in simple cases: Lifshitz,

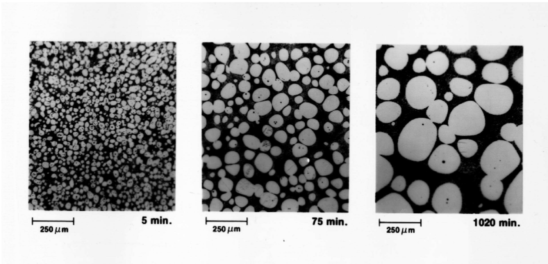

Figure 2: Experimental observation of round particles

Slyozov [LiSl61] and Wagner [Wag61] found a $t^{1/3}$-law for the average growth rate of the particles. The two latter stages are assumed to be driven by diffusion.

The materials which are modelled are solid materials, the diffusion process which is described here is therefore only very slow. Observable changes might happen only after hours, days or even years. This behaviour is also called material aging.

To understand this separating process is thus of high technological importance, since one would like to control or slow down the separation process and maybe even stop it. The alloy usually looses its desired properties at a certain coarse rate. So, in order to make good predictions of the aging behaviour one aim was to develop reliable mathematical models. We are going to study two types of models.

One model has been proposed by Mullins and Sekerka. It is assumed that after the spinodal decomposition every point in the material piece $\Omega \subset \mathbb{R}^d$ can be identified uniquely either as material corresponding to $+1$ or as the one corresponding to -1. This means we have a function $\rho\colon \Omega \to \{\pm 1\}$ with only two possible values. If the boundary set

$$\Gamma := \partial\{\rho = 1\} \cap \Omega = \partial\{\rho = -1\} \cap \Omega$$

is smooth enough, a harmonic potential w is determined by having the mean curvature κ of Γ as boundary values:

$$\begin{aligned} \Delta w &= 0, && \text{in } \Omega \setminus \Gamma, \\ w &= \kappa, && \text{on } \Gamma. \end{aligned}$$

Then the interface moves according to the normal velocity law

$$V = [\nabla w]_-^+ \cdot \nu_\Gamma = (\nabla w^+ - \nabla w^-) \cdot \nu_\Gamma,$$

i.e. by the normal part of the difference of the gradient of w at the interface. The boundary value condition for w is also called Gibbs-Thomson law. The importance of this condition originates from thermo-dynamics: the laws of thermo-dynamics are fulfilled for this model. Such models which are based on evolving hypersurfaces are categorised as sharp-interface models, since the interface is represented by a $(d-1)$-dimensional surface.

A different approach has been made by Cahn and Hilliard. They described the phases by a concentration function which assumes different values in the respective phases, here ± 1. But the function is not allowed to simply jump between these values, but it has to interpolate the values smoothly. This means that the boundary will not be represented by a $(d-1)$-dimensional surface, but more as a smeared out version of it. The formulation incorporates a concentration function ρ and a chemical potential w, where the diffusion of the mass is driven by the gradient of the potential:

$$\begin{aligned} \partial_t \rho &= \Delta w, \\ w &= -\varepsilon \Delta \rho + \tfrac{1}{\varepsilon} \Psi'(\rho). \end{aligned}$$

Such so-called phase-field formulations are generally easier to work with analytically and numerically. This is due to the topological change in the sharp-interface model, whenever two particles merge, one big brakes into two or one disappears.

The above two models have been extensively studied, but when compared with experimental observations, it became apparent that they have certain real-life limitations: they would only model cases where the particles are round, the larger ones always grow at the cost of the smaller ones, which can be explained by the isotropic structure of the equations. This is sufficient for Ni-Al-Si alloys, see [MEPC94], but when looking at alloys as Ni-Al which were studied in [MaAr93], the particles can

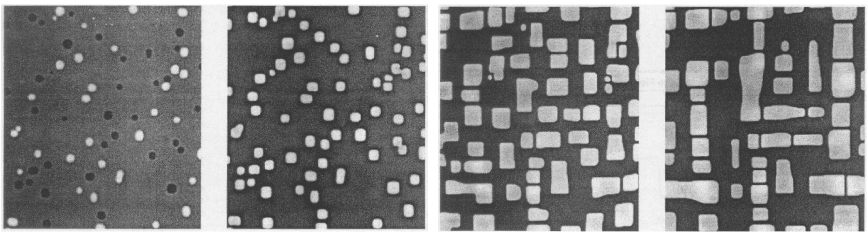

Figure 3: Experimental observations of rectangular particles

also show a different behaviour: particles can have an edgy, rectangular shape, smaller ones don't necessarily shrink and vanish, particles might align and a slow-down of the whole separating process is possible, see Figure 3. This behaviour was assumed to origin from elastic effects and indeed numerical simulations have indicated that elasticity can explain these different features of alloys.

The main part of this work is to relate the elastically extended versions of the phase-field and the sharp-interface model. The coupled system will be modelled in a quasi-stationary way: the concentration or the free boundary Γ will be driven by a diffusion via a chemical potential. But it is the chemical potential which will have some additional elastic terms. The deformation vector function which describes the elastic properties of the material is assumed to be a stationary solution of the mechanical system, since the mechanical equilibrium is attained on a much faster scale compared to the diffusion process. It is shown that weak solutions of the phase-field model converge to an appropriately chosen weak solution of the sharp-interface model. Special care has to be taken for the Gibbs-Thomson law which includes the mean curvature. Curvature usually assumes a smooth geometry, but in the asymptotic limit of phase-field solutions this cannot be guaranteed. Therefore the notion of mean curvature has to be weakened. Here we replace the curvature term by using varifolds which are Radon measure on the Grassmanian

$$G(\bar{\Omega}) := \bar{\Omega} \times \mathbb{P}^{d-1} = \bar{\Omega} \times \left(\mathbb{S}^{d-1}/\{\pm 1\}\right).$$

For bounded $\Omega \subset \mathbb{R}^d$ the Grassmanian is compact and as Radon measures the space of varifolds inherits the $(C^0(G(\bar{\Omega})))^*$-structure and compactness. Moreover the first variation of a varifold is established and generalises the curvature of $(d-1)$-dimensional objects.

In the first chapter the elastically extended models are presented. Here we apply homogeneous elasticity theory including misfits. The weak solution of the phase-field model and some properties, most important the gradient flow structure and an energy functional, are established. The solution of the phase-field model corresponds to a gradient flow to a respective energy functional. In fact it is the gradient flow structure which will guarantee through a time discretisation the existence of an evolving solution for given initial values.

The second chapter introduces the notations and presents ideas of geometric measure theory which is used in this work. It is explained how the curvature is included in this measure-theoretical notion and in which case the varifold is in fact a countably rectifiable set with a nearly C^1-structure.

After defining the generalised solution of the sharp-interface model, the third chapter states and proves the main result: the weak solutions of the phase-field model from the first chapter converge to a generalised solution of the sharp-interface model. Convergences of concentration, chemical potential and deformation vector function are derived in respective function spaces by a priori estimates. Moreover the term describing the interface energy in the phase-field model is identified and it is shown in Subsection 3.2.6 that this term converges to a Radon measure. A tedious part is to identify a varifold in the $\varepsilon \to 0$-limit process, for which an estimate of the so-called discrepancy measure is shown. This result also yields the existence of a global in time solution for the sharp-interface model in the generalised sense of Chapter 3. See explanations in Subsection 3.1.1 for further information. An overview of comparable results and works is given in Section 3.3. To our knowledge this is the first rigorous result for the elastically extended Cahn-Hilliard system, also called Cahn-Larché system. That is for given, admissible initial values the solutions of the phase-field model derived in Chapter 1 will converge to a generalised solution without any further assumption on smoothness or energy estimates.

For the last chapter we return to one of the main original questions from the material science point of view:

> Is it possible to find alloys which don't show the phase separation as much as other alloys or which maybe even show an *inverse coarsening* behaviour?

We study one dimensional and rotation-symmetric cases and indeed a few possible situations are found where an inverse coarsening is expected.

I would like to thank my supervisor Prof. H. Garcke for introducing me to this interesting field of partial differential equations, geometric measure theory and geometry and for the constant support over the years. I am very grateful to Matthias Röger for many helpful discussions on geometric measure theory.

1 Models

In our setting we always choose $\Omega \subset \mathbb{R}^d$ to be an open, bounded domain with $C^{2,\alpha}$-boundary for some $\alpha \in (0,1)$. The dimension d is restricted to at most 3. We start with a short review of elasticity theory and present the elastically extended phase-field and sharp-interface models. The gradient flow structure of the phase-field model will be discussed with the subsequent existence theory of weak solutions of the phase-field model.

1.1 Introduction to mechanics

Among the different models of elasticity we choose the so-called linear elasticity. Elastic effects are described using a *deformation field* $\mathbf{u}\colon \Omega \to \mathbb{R}^d$. The idea is that Ω is a *reference state*. For each material point $x \in \Omega$ the position x itself corresponds to the undeformed body state and $x + \mathbf{u}(x)$ refers to the position in the deformed body. The mechanical forces which are observed in the deformed state are described by the *strain tensor* $\mathcal{E}$, which in its full form is given by

$$\mathcal{E}(\mathbf{u}) = \tfrac{1}{2}(\nabla\mathbf{u} + \nabla\mathbf{u}^T + \nabla\mathbf{u}\nabla\mathbf{u}^T).$$

In the case of phase separation the deformation will have a rather small gradient, which means that overall the appearing deformation is not large – we are not modelling any macroscopic phenomenon as bending a steel bar. Therefore we restrict ourselves to the *linearised strain tensor*

$$\mathcal{E}(\mathbf{u}) = \tfrac{1}{2}(\nabla\mathbf{u} + \nabla\mathbf{u}^T). \tag{1.1}$$

The *elastic energy density* W is assumed to be a quadratic form

$$W(\rho, \mathcal{E}) = \tfrac{1}{2}\big(\mathcal{E} - \mathcal{E}^*\rho\big) : \mathcal{C}\big(\mathcal{E} - \mathcal{E}^*\rho\big) \tag{1.2}$$

with a symmetric and positive definite, homogeneous *elasticity tensor* $\mathcal{C}$. So, we can describe $\mathcal{C}$ as $\mathcal{C} = (\mathcal{C}_{ijkl})_{ijkl}$ with

$$\mathcal{C}(A) = \Big(\sum_{k,l=1}^{d} \mathcal{C}_{ijkl}A_{kl}\Big)_{ij}, \quad \mathcal{C}_{ijkl} = \mathcal{C}_{klij}, \quad \mathcal{C}_{ijkl} = \mathcal{C}_{jikl}. \tag{1.3}$$

Here ,we use ':' for the inner product of matrices:

$$A : B := \operatorname{tr}(A^T B) = \sum_{i,j} A_{ij}B_{ij}.$$

We call $\mathcal{E}^*\rho$ the *eigenstrain* corresponding to ρ which describes the energetically favourable strain at concentration ρ. A difference of these eigenstrains, which are given and symmetric, is called misfit. This is the reason why the elasticity can have a noticeable effect on the diffusion process. If $\mathcal{C}$ depends on the concentration ρ, the elasticity is called *inhomogeneous*, but we restrict ourself to the *homogeneous elasticity* case, see discussion at the end of the chapter. For the theory we are going to present in this work we use the following properties of homogeneous elasticity, which follow by (1.2): there exists a constant $C > 0$ such that

$$\begin{aligned} &W \in C^1(\mathbb{R}\times\mathbb{R}^{d\times d}, \mathbb{R}) \quad \text{such that for all } \rho \in \mathbb{R},\ \mathcal{E} \in \mathbb{R}^{d\times d} \\ &\quad |W(\rho, \mathcal{E})| \leq C(1 + |\rho|^2 + |\mathcal{E}|^2), \\ &\quad |W_{,\mathcal{E}}(\rho, \mathcal{E})| \leq C(1 + |\rho| + |\mathcal{E}|), \\ &\quad |W_{,\rho}(\rho, \mathcal{E})| \leq C(1 + |\rho| + |\mathcal{E}|). \end{aligned} \tag{1.4}$$

and $W_{,\mathcal{E}}$ is a sum of terms which depend either on ρ or $\mathcal{E}$, as it is used in Proposition 1.7.

By the symmetry and positive definiteness of the elasticity tensor $\mathcal{C}$ it follows that $W(\rho, \mathcal{E})$ only depends on the symmetric part of $\mathcal{E} \in \mathbb{R}^{d\times d}$

$$W(\rho, \mathcal{E}) = W(\rho, \mathcal{E}^T)$$

and that $W_{,\mathcal{E}}$ is strongly monotone, i.e. there exists a constant $c_1 > 0$ such that

$$(W_{,\mathcal{E}}(\rho, \mathcal{E}_2) - W_{,\mathcal{E}}(\rho, \mathcal{E}_1)) : (\mathcal{E}_2 - \mathcal{E}_1) \geq c_1|\mathcal{E}_2 - \mathcal{E}_1|^2. \tag{1.5}$$

The mechanical equilibrium is attained on a much faster time scale compared to the concentration which changes by diffusion. This is why we assume that the mechanical equilibrium is attained instantaneously, so that the equation for the mechanics (1.6) does not involve any time derivatives and we hence consider at each time $t > 0$ the *quasi-stationary* system:

$$\operatorname{div} S = \operatorname{div} W_{,\mathcal{E}}(\rho, \mathcal{E}(\mathbf{u})) = 0 \tag{1.6}$$

where $S = S(\rho, \mathcal{E}) = W_{,\mathcal{E}}(\rho, \mathcal{E})$ is the *stress tensor*.

For definiteness we demand the deformation field $\mathbf{u}$ to be in $\mathrm{X}_{\mathrm{ird}}^{\perp}$ with

$$\begin{aligned} \mathrm{X}_{\mathrm{ird}} :=& \{\mathbf{u} \in H^{1,2}(\Omega, \mathbb{R}^d) \mid \text{ there exist } b \in \mathbb{R}^d \text{ and a skew symmetric} \\ &\qquad A \in R^{d\times d} \text{ such that } \mathbf{u}(x) = b + Ax\} \\ =& \{\mathbf{u} \in H^{1,2}(\Omega, \mathbb{R}^d) \mid \mathcal{E}(\mathbf{u}) = 0\} \end{aligned} \tag{1.7}$$

and $\mathrm{X}_{\mathrm{ird}}^{\perp}$ is the space perpendicular to the infinitesimally rigid deformations $\mathrm{X}_{\mathrm{ird}}$ where perpendicular is meant with respect to the $H^{1,2}$-inner product. We remark that the elastic energy depends on $\mathbf{u}$ only through $\mathcal{E}(\mathbf{u})$ and hence the infinitesimally rigid part of $\mathbf{u}$, i.e. the part in $\mathrm{X}_{\mathrm{ird}}$, has no influence on the evolution of ρ. One important property of $\mathrm{X}_{\mathrm{ird}}^{\perp}$, which we will use later for definiteness, is that the *Korn inequality*

$$\|\mathbf{u}\|_{H^{1,2}(\Omega)} \leq \tilde{C}\|\mathcal{E}(\mathbf{u})\|_{L^2(\Omega)}$$

holds for all $\mathbf{u} \in \mathrm{X}_{\mathrm{ird}}^{\perp}$ for some constant $\tilde{C} > 0$ (cf. A.3). In particular we will obtain using (1.5) and an energy argument that $\mathbf{u} \in \mathrm{X}_{\mathrm{ird}}^{\perp}$ is uniquely determined by (1.6) and a stress-free boundary condition

$$S\nu = 0.$$

For more detailed information on models of elasticity we refer to [Gur72], [Cia88] and [Brae91].

1.2 The phase-field and the sharp-interface model

The extension of the Cahn-Hilliard model by elasticity was proposed by Cahn and Larché in [CahLar82]. It is based on the Ginzburg-Landau type energy

$$\mathbf{E}^{\varepsilon}_{\mathbf{pf}}(\rho, \mathbf{u}) = \int_{\Omega} \left(\frac{\varepsilon}{2} |\nabla \rho|^2 + \frac{1}{\varepsilon} \Psi(\rho) + W(\rho, \mathcal{E}(\mathbf{u})) \right) \tag{1.8}$$

for $\rho \in H^{1,2}(\Omega)$ and $\mathbf{u} \in H^{1,2}(\Omega, \mathbb{R}^d)$, where $\varepsilon > 0$ is a small parameter related to the thickness of the diffuse interface, ρ is a scaled concentration difference, Ψ is a smooth double well potential, which we take to be of the form

$$\Psi(\rho) \in C^2(\mathbb{R}) \quad s.t.\ \Psi(\pm 1) = 0, \Psi(\rho) > 0 \quad \forall\, \rho \neq \pm 1, \tag{1.9}$$

$$\exists c_0 > 0 : \Psi''(\rho) \geq c_0 |\rho|^{p-2} \quad \forall |\rho| \geq 1 - c_0 \tag{1.10}$$

for some $p > 2$ or $p \in (2, 4]$ in the 3-dimensional case. The case $p = 2$ is not applicable due to Lemma 3.18. One example of such a potential would be

$$\Psi(\rho) = (\rho^2 - 1)^2 (\rho^2 + 1)^{p/2-2} \tag{1.11}$$

where the case $p = 4$ is the most typical one.

Remark.

(i) In other words we require that Ψ has roots of exactly order 2 in ± 1. For values outside $(-1, 1)$ the function Ψ grows with order p. There are no restrictions about other local minima (with positive value) than those two or about any symmetry. This is of concern, if one analyses the behaviour of a single phase-field system, but not in the asymptotic limit we are interested in. Note that (1.10) does not apply for potentials as $\Psi(\rho) = (1 - \rho^2)^p$. The convexity of our potential will become important later in Lemma 3.7 when we apply the Modica ansatz.

(ii) The conditions on Ψ are chosen in such a way that admissible concentration functions will be in $L^p(\Omega)$. We will derive this property and also $\Psi'(\rho) \in L^2(\Omega)$ later using Sobolev-embeddings, see Lemma 1.5. This will be of importance in Lemma 3.18 where we have to meet a certain integrability condition, see also Lemma 3.23. It is again Lemma 3.18 where we have to exclude $p = 2$.

In the diffuse interface model the Cahn-Larché system can be derived as evolution problem related to (1.8):

$$\partial_t \rho = \Delta w \qquad \text{in } \Omega \times (0, T), \tag{1.12}$$

$$w = \frac{\delta \mathbf{E}^{\varepsilon}_{\mathbf{pf}}}{\delta \rho} = -\varepsilon \Delta \rho + \tfrac{1}{\varepsilon} \Psi'(\rho) + W_{,\rho}(\rho, \mathcal{E}(\mathbf{u})) \qquad \text{in } \Omega \times (0, T), \tag{1.13}$$

$$\operatorname{div} S = \operatorname{div} \frac{\delta \mathbf{E}^{\varepsilon}_{\mathbf{pf}}}{\delta \mathcal{E}} = 0 \qquad \text{in } \Omega \times (0, T), \tag{1.14}$$

where w is the chemical potential. See Section 1.3 below for more explanations of the derivation of the equations. As we will see later this evolution problem incorporates the mass conservation: in our model the mass $\int_\Omega \rho dx$ does not change over time.

If for the sharp-interface model the phases are given by a binary function ρ and the interface $\Gamma := \partial\{\rho = 1\} \cap \Omega = \partial\{\rho = -1\} \cap \Omega$ is smooth enough, then the energy in this case is given by

$$\mathbf{E_{si}}(\Gamma, \mathbf{u}) = 2\sigma\,\mathcal{H}^{d-1}(\Gamma) + \sum_{k=\pm 1} \int_{\Omega_k} W(k, \mathcal{E}(\mathbf{u}))\,dx \tag{1.15}$$

where $\sigma > 0$ is a surface energy constant. The notation $\mathcal{H}^{d-1}(.)$ denotes the $(d-1)$-dimensional Hausdorff measure and $\Omega_{\pm 1}$ are the distinct regions occupied by the two phases. The surface energy density σ is related to the double well potential of the phase-field model (1.9) by the formula

$$\sigma = \tfrac{1}{2} \int_{-\infty}^{\infty} \tfrac{1}{2}(z'(y))^2 + \Psi(z(y))dy, \tag{1.16}$$

where z is the solution of

$$-z'' + \Psi'(z) = 0 \qquad \text{with} \lim_{y\to\pm\infty} z(y) = \pm 1.$$

By a reparametrisation σ can be expressed as

$$\sigma = \int_{-\infty}^{\infty} z'(y)\sqrt{\Psi(z(y))/2}\,dy = \int_{-1}^{1} \sqrt{\Psi(z)/2}\,dz. \tag{1.17}$$

In the concrete example $\Psi(\rho) = (\rho^2 - 1)^2$ the surface energy results to

$$\sigma = \int_{-1}^{1} \sqrt{(z^2-1)^2/2}\,dz = \frac{2}{3}\sqrt{2}.$$

Remark. In a more general setting (for instance describing multi-phase systems using multi-well potentials) σ represents the distance between the two minimal phases of the chemical potential (generally one has to specify two of the minima states, but here we have only $\rho = \pm 1$ as minima, so we only have one distance to deal with). Then the definition is

$$\sigma(\rho_+, \rho_-) := \inf\left\{ \tfrac{1}{2} \int_{-\infty}^{\infty} \left|\gamma'(y)\right| \sqrt{\Psi(\gamma(y))/2}dy \mid \lim_{y\to\pm\infty} \gamma(y) = \rho_\pm \right\}.$$

So, in the multi-phase case one has also to handle the choice of path connecting two minima. See [GaNeSt04] for some discussion about multi-phase systems.

Remark. We can rewrite the energy of the sharp interface model by using a binary concentration function with bounded perimeter:

$$\mathbf{E_{si}}(\rho, \mathbf{u}) = 2\sigma\,\mathcal{H}^{d-1}(\partial\{\rho = 1\}) + \int_\Omega W(\rho, \mathcal{E}(\mathbf{u}))\,dx \tag{1.18}$$

for $\rho \in BV(\Omega, \{-1, 1\})$ and $\mathbf{u} \in H^{1,2}(\Omega, \mathbb{R}^d)$. This formulation is more convenient to state the Γ-convergence of the energy functionals, see Theorem 1.1.

The evolution problem related to the sharp interface energy is a modified Mullins-Sekerka problem

$$\Delta w = 0 \qquad \text{in } \Omega_-(t) \text{ and } \Omega_+(t), \tag{1.19}$$

$$V = \tfrac{1}{2}[\nabla w]_-^+ \cdot \nu \qquad \text{on } \Gamma(t), \tag{1.20}$$

$$w = \sigma\kappa + \tfrac{1}{2}\nu^T[W\,\mathbf{id} - (\nabla\mathbf{u})^T S]_-^+\nu \qquad \text{on } \Gamma(t), \tag{1.21}$$

$$\operatorname{div} S = 0 \qquad \text{in } \Omega_-(t) \text{ and } \Omega_+(t), \tag{1.22}$$

$$[S\nu]_-^+ = [\mathbf{u}]_-^+ = 0,\ [w]_-^+ = 0 \qquad \text{on } \Gamma(t)$$

where $\Omega_-(t)$ and $\Omega_+(t)$ are the regions occupied by the phases at time t, $\Gamma(t)$ is the interface separating these regions, ν is the unit normal along the interface pointing into Ω_+, V is the normal velocity of the interface and $[\,.\,]_-^+$ denotes the jump of the quantity in the brackets across the interface, e.g. $[w]_-^+ = w^+ - w^-$. κ is the mean curvature of $\Gamma(t)$ with the sign convention that κ is positive, if $\Gamma(t)$ is curved in the direction of ν, i.e. the sphere with outer normal has positive curvature. In contrast to other definitions the mean curvature is taken here to be the sum of the principle curvatures with respect to the outer normal. The first two equations are classical laws describing quasi-static diffusion driven by a chemical potential w. The third equation is the modified Gibbs-Thomson equation stating that the system is in local thermo-dynamical equilibrium.

Since we want to restrict our analysis to closed systems, we take homogeneous Neumann boundary conditions. In the phase-field model this means that we have on $\partial\Omega$

$$\nabla\rho \cdot \nu_\Omega = \nabla w \cdot \nu_\Omega = 0, \quad S\nu_\Omega = 0, \tag{1.23}$$

where ν_Ω denotes the outer unit normal of Ω. In the sharp interface model the condition for the concentration changes to an angle condition for the interface, so the boundary conditions for the sharp interface model are

$$\angle(\Gamma(t), \partial\Omega) = 90^\circ, \quad \nabla w \cdot \nu_\Omega = 0, \quad S\nu_\Omega = 0. \tag{1.24}$$

Comparing the two systems of equations some analogues can be found by simple formal arguments. The weak formulation of (1.12) is of the same form as (1.19) and (1.20) written in distributional sense. The *Eshelby tensor* $\frac{1}{2}\nu^T[W\,\mathbf{id} - (\nabla\mathbf{u})^T S]_-^+\nu$ corresponds to $W_{,\rho}$ in (1.13) which means that $(-\varepsilon\Delta\rho + \frac{1}{\varepsilon}\Psi'(\rho))$ includes the curvature information. Moreover, as we will see later in Proposition 3.2 (ii) and Subsection 3.2.6, the function

$$e^\varepsilon(\rho) := \frac{\varepsilon}{2}|\nabla\rho|^2 + \frac{1}{\varepsilon}\Psi(\rho)$$

will converge to the $(d-1)$-dimensional measure of the sharp interface, therefore it is called *surface energy density*. The term $-\varepsilon\Delta\rho + \frac{1}{\varepsilon}\Psi'(\rho)$ in equation (1.13) is the variational derivative of $e^\varepsilon(\rho)$. Recall that the variation of the area measure functional

$$A(\Gamma) = \int_\Gamma 1\, d\mathcal{H}^{d-1}$$

of a smooth hypersurface Γ is given by its curvature:

$$\frac{\delta A}{\delta \Gamma}(\zeta) = -\int_{\Gamma} \zeta \cdot \nu_{\Gamma} \kappa_{\Gamma} \, d\mathcal{H}^{d-1} = \int_{\Gamma} \mathrm{div}_{\Gamma} \, \zeta \, d\mathcal{H}^{d-1}$$

for all $\zeta \in C_0^1(\Gamma, \mathbb{R}^d)$. This shows the relations between the terms of (1.12)–(1.14) and (1.19)–(1.22). Moreover, the energies of the phase-field and sharp interface models are related by a Γ-limit:

Theorem 1.1.

$$\mathbf{E}_{\mathbf{pf}}^{\varepsilon} \xrightarrow{\Gamma} \mathbf{E}_{\mathbf{si}}. \tag{1.25}$$

In detail this means that

(i) for every sequence $(\rho^{\varepsilon_k}, \mathbf{u}^{\varepsilon_k}) \in \mathcal{M} \times \mathrm{X}_{\mathrm{ird}}^{\perp}$ *such that* $\rho^{\varepsilon_k} \to \rho$ *in* $L^1(\Omega)$ *and* $\mathbf{u}^{\varepsilon_k} \to \mathbf{u}$ *in* $L^2(\Omega, \mathbb{R}^d)$ *as* ε_k *tends to zero, it holds*

$$\mathbf{E}_{\mathbf{si}}(\rho, \mathbf{u}) \leq \liminf_{k \to \infty} \mathbf{E}_{\mathbf{pf}}^{\varepsilon_k}(\rho^{\varepsilon_k}, \mathbf{u}^{\varepsilon_k}). \tag{1.26}$$

(ii) for any $(\rho, \mathbf{u}) \in L^1(\Omega) \times \mathrm{X}_{\mathrm{ird}}^{\perp}$ *and sequence* $\varepsilon_k \to 0$ *there exists a sequence* $(\rho^{\varepsilon_k}, \mathbf{u}^{\varepsilon_k}) \in \mathcal{M} \times \mathrm{X}_{\mathrm{ird}}^{\perp}$ *with* $\rho^{\varepsilon_k} \to \rho$ *in* $L^1(\Omega)$ *and* $\mathbf{u}^{\varepsilon_k} \to \mathbf{u}$ *in* $L^2(\Omega, \mathbb{R}^d)$ *as* ε_k *tends to zero, such that*

$$\mathbf{E}_{\mathbf{si}}(\rho, \mathbf{u}) \geq \limsup_{k \to \infty} \mathbf{E}_{\mathbf{pf}}^{\varepsilon_k}(\rho^{\varepsilon_k}, \mathbf{u}^{\varepsilon_k}). \tag{1.27}$$

We denote by $\mathcal{M}$ the restriction of $H^{1,2}(\Omega)$ to a fixed total mass $\int_{\Omega} \rho = m_0 |\Omega|$, see (1.43).

Proof. This has been shown in [Gar00]. □

The concept of Γ-limit is to relate the energy functionals of the phase-field model and the sharp interface model as $\varepsilon \to 0$. One important feature of the Γ-limit is that for any sequence of minimisers of $\mathbf{E}_{\mathbf{pf}}^{\varepsilon}$ any limit point of the sequence, i.e. any cluster point, is a minimiser of the limit functional $\mathbf{E}_{\mathbf{si}}$. This means that stationary solutions of the Cahn-Larché system converge to a stationary solution of the sharp interface model. For a brief introduction to Γ-convergence see for example [Alb00].

More remarks about the relation of Γ-limit and the result of the present work are made in Subsection 3.3.

1.3 Gradient flow structure and time discretisation

We begin with the general notion of gradient flows. We take a differentiable manifold $(\mathcal{M}, (.,.)_{\mathcal{M}})$ and a differentiable energy function $\mathbf{E} \colon \mathcal{M} \to [0, \infty]$. We can define the variational derivative of this energy function at a point $u \in \mathcal{M}$ with respect to some direction $v \in T_u\mathcal{M}$ by

$$\frac{\delta \mathbf{E}}{\delta u}(u)(v) = \frac{d}{dt}\Big|_{t=0} \mathbf{E}(\gamma_v^u(t)), \tag{1.28}$$

where $\gamma_v^u\colon (-\delta,\delta) \to \mathcal{M}$ is a curve representing $v \in T_u\mathcal{M}$, i.e. $\gamma_v^u(0) = u,\ \partial_t\gamma_v^u(0) = v$. This means that $\frac{\delta \mathbf{E}}{\delta u}$ is a mapping $\mathcal{M} \to (T\mathcal{M})'$ into the dual space of the tangential bundle, i.e.

$$\frac{\delta \mathcal{E}}{\delta u}(u_0) \in (T_{u_0}\mathcal{M})' \quad \text{for } u_0 \in \mathcal{M}.$$

By the representation theorem by Riesz we have an equivalent element in $T\mathcal{M}$ which we call gradient:

$$(\operatorname{grad} \mathbf{E}(u), v)_{\mathcal{M}} = \frac{\delta \mathbf{E}}{\delta u}(u)(v) \quad \forall v \in T_u\mathcal{M}. \tag{1.29}$$

If we have a time-dependent $u : I := [0,T] \to \mathcal{M}$, we now say that u is a *gradient flow* to $\mathbf{E}$ in $\mathcal{M}$, if

$$\partial_t u = -\operatorname{grad} \mathbf{E}(u). \tag{1.30}$$

If u evolves as gradient flow to $\mathbf{E}$ in $\mathcal{M}$, we have as immediate consequence the energy decay:

Lemma 1.2. *For a gradient flow u to the energy function $\mathbf{E}$ in $\mathcal{M}$, the energy dissipates in the following way:*

$$\frac{d}{dt}\mathbf{E}(u(t)) = -\|\partial_t u\|_{\mathcal{M}}^2 \leq 0 \qquad \textit{for all } t \in I. \tag{1.31}$$

Moreover it holds for all $t \in I$

$$\mathbf{E}(u(t)) + \int_0^t \|\partial_t u\|_{\mathcal{M}}^2 = \mathbf{E}(u(0)). \tag{1.32}$$

Proof. The estimate is based on the identity

$$\frac{d}{dt}\mathbf{E}(u(t)) = \frac{\delta \mathbf{E}}{\delta u}(u)\partial_t u = (\operatorname{grad} \mathbf{E}(u), \partial_t u)_{\mathcal{M}} = -\|\partial_t u\|_{\mathcal{M}}^2. \tag{1.33}$$

□

Combining equations (1.29) and (1.30), we finally obtain the *gradient flow equation* in the variational description for some initial data u^0:

$$-(\partial_t u(s), v(s))_{\mathcal{M}} = \frac{\delta \mathbf{E}}{\delta u}(u(s))(v(s)) \quad \forall\, s \in I, \forall\, v \in \{v\colon I \to T\mathcal{M} \mid v(s) \in T_{u(s)}\mathcal{M}\} \tag{1.34}$$

$$\text{and} \qquad u(0) = u^0. \tag{1.35}$$

So, given the energy function $\mathbf{E}$ in $\mathcal{M}$ we look for a time-dependent mapping $u\colon I \to \mathcal{M}$ which solve (1.34) and (1.35). Since the gradient is the direction of steepest ascent, this means that the system tries to minimise the energy function by moving in the direction of steepest descent within the energy landscape which we imagine to be the graph of $\mathbf{E}$ over $\mathcal{M}$.

The existence of smooth solutions which are gradient flows of the energy cannot be guaranteed though. In some cases this can be overcome by a property of gradient flow equations: they inhibit a natural *time discretisation*.

We divide the time interval $I = \cup_i [i\Delta t, (i+1)\Delta t]$ for $i = 0, ..., M$. We call u^j the value of u at time $j\,\Delta t \in I$. Then the next value $u^i, i = j+1$ is chosen by minimising the energy penalised by a time-difference term:

$$u^i = \arg\min_{u\in\mathcal{M}} \left(\mathbf{E}(u) + \frac{1}{2\Delta t}\|u - u^{i-1}\|^2_{\mathcal{M}} \right). \tag{1.36}$$

If the time-discrete energy, i.e. $\mathbf{E}(u)+\frac{1}{2\Delta t}\|u-u^{i-1}\|^2$, is coercive, then the existence of a minimiser u^i can be guaranteed. Here an upper bound for the time-step Δt usually arises.

A direct consequence of (1.36) is a time-discrete version of the energy decay (1.32)

$$\mathbf{E}(u^i) + \frac{1}{2\Delta t}\|u^i - u^{i-1}\|^2_{\mathcal{M}} = \mathbf{E}(u^{i-1}). \tag{1.37}$$

The variational ansatz of above minimisation problem recovers a time-discrete version of the gradient flow equation (1.34)

$$-\frac{1}{\Delta t}\left(u^i - u^{i-1}, v\right)_{\mathcal{M}} = \frac{\delta \mathbf{E}}{\delta u}(u^i)(v) \qquad \forall\, v \in T_{u^i}\mathcal{M}. \tag{1.38}$$

Finally, one has to show that the time-discrete solution converges for infinitesimally small time-steps to a weak solution of the gradient flow equation (1.34).

Now, we apply this ansatz to our energy functional of the Cahn-Larché system

$$\mathbf{E}^{\varepsilon}_{\mathbf{pf}}(\rho, \mathbf{u}) = \int_\Omega \left(\frac{\varepsilon}{2}|\nabla\rho|^2 + \frac{1}{\varepsilon}\Psi(\rho) + W(\rho, \mathcal{E}(\mathbf{u})) \right). \tag{1.39}$$

We notice that it depends both on a concentration and on a deformation field. This means we have two different variational derivatives of our energy functional. Experiments have shown that the mechanical equilibrium is reached by far faster than the diffusion process. It is thus assumed that the mechanical equilibrium is in fact attained instantaneously, effectively we have

$$\mathbf{u} = \mathbf{u}(\rho).$$

The equilibrium state is described by

$$\operatorname{div} \frac{\delta \mathbf{E}^{\varepsilon}_{\mathbf{pf}}}{\delta \mathbf{u}} = \operatorname{div} W_{\mathcal{E}} = 0 \tag{1.40}$$

which states that at each point in our material sample the mechanical forces cancel each other out, following Newton's law of annihilation of forces. We describe the evolution of the concentration as a diffusion process and use the gradient flow description as introduced above:

$$\frac{\delta \mathbf{E}^{\varepsilon}_{\mathbf{pf}}}{\delta \rho}(v) = -\left(\partial_t \rho, v\right)_{\mathcal{M}} \qquad \forall v \in T_\rho\mathcal{M}. \tag{1.41}$$

We have to define the function spaces with the respective metric or norms. Here, we choose the manifold to be some appropriate Sobolev space, so that later we can guarantee the existence of solutions. As introduced in Section 1.1 we choose the manifold $\widetilde{\mathcal{M}}$ for the deformation field to be $\mathrm{X}_{\mathrm{ird}}$:

$$\widetilde{\mathcal{M}} := \mathrm{X}_{\mathrm{ird}}^{\perp} = \{\mathbf{u} \in H^{1,2}(\Omega, \mathbb{R}^d) \mid \mathcal{E}(\mathbf{u}) = 0\}, \tag{1.42}$$

and for the concentration function we are only interested in functions which have a fixed mean value, so we model the mass preserving property of the separation phenomenon:

$$\mathcal{M} := \mathcal{M}_{m_0} := \big\{\rho \in H^{1,2}(\Omega) \mid \int_\Omega \rho = m_0|\Omega|\big\}, \tag{1.43}$$

for a constant $m_0 \in (-1, 1)$. As metric on $\mathcal{M}$ we don't take the $H^{1,2}$-Norm, but the $H^{-1,2}$-Norm which we derive in the following: The manifold $\mathcal{M}$ as defined above has the tangential structure

$$T_\rho\mathcal{M} = H_0^{1,2}(\Omega) := \big\{v \in H^{1,2}(\Omega) \mid \int_\Omega v = 0\big\}. \tag{1.44}$$

Then we call the dual space of $T_\rho\mathcal{M}$ with respect to the $H^{1,2}$-Norm

$$H^{-1,2}(\Omega) := (T_\rho\mathcal{M})^*. \tag{1.45}$$

Note that every functional $F \in H^{-1,2}(\Omega) = H_0^{1,2}(\Omega)^*$ can be extended to a continuous functional on the entire $H^{1,2}(\Omega)$ by setting

$$F(c) := 0 \qquad \forall\, c \in \mathbb{R}. \tag{1.46}$$

For a functional $F \in H^{-1,2}(\Omega)$ the Poisson problem

$$-\Delta w = F \qquad \text{in } \Omega, \tag{1.47}$$

$$\frac{\partial w}{\partial \nu} = 0 \qquad \text{on } \partial\Omega \tag{1.48}$$

can be uniquely solved in a weak sense, so we can define the solution operator

$$(-\Delta_0)^{-1} : H^{-1,2}(\Omega) \to H_0^{1,2}(\Omega), \tag{1.49}$$

$$F \mapsto w := (-\Delta_0)^{-1}F. \tag{1.50}$$

Remark. This follows by application of the Poincaré-inequality and the Lax-Milgram theorem. We can apply the Poincaré-inequality, because $T_\rho\mathcal{M}$ is not the full $H^{1,2}(\Omega)$ space, but is restricted to the subspace with mean value zero.

Now, for two functionals $F_1, F_2 \in H^{-1,2}(\Omega)$ we define

$$\begin{aligned}(F_1, F_2)_{-1} :&= \int_\Omega \nabla\left((-\Delta_0)^{-1}F_1\right) \cdot \nabla\left((-\Delta_0)^{-1}F_2\right) = \int_\Omega \nabla w_1 \cdot \nabla w_2 \\ &= F_1((-\Delta_0)^{-1}F_2) = F_2((-\Delta_0)^{-1}F_1) = F_1(w_2) = F_2(w_1)\end{aligned} \tag{1.51}$$

for $w_i = (-\Delta_0)^{-1} F_i$.

Since the operator is injective, we see that $(.,.)_{-1}$ is a scalar product on

$$H_0^{1,2}(\Omega) \subset \{v \in L^2(\Omega) \mid \int_\Omega v = 0\} \subset H^{-1,2}(\Omega).$$

Note that we have the second embedding by setting

$$F_f(\zeta) := \int_\Omega f\,\zeta\,dx \quad \forall \zeta \in H_0^{1,2}(\Omega) \tag{1.52}$$

for $f \in \{v \in L^2(\Omega) \mid \int_\Omega v = 0\}$.

Now we apply the time-discretisation ansatz (1.36), i.e. we look for the minimiser

$$\rho^i := \arg\min_{\rho \in \mathcal{M}} \left(\mathbf{E}^\varepsilon_{\mathbf{pf}}(\rho, \mathbf{v}(\rho)) + \frac{1}{2\Delta t} \|\rho - \rho^{i-1}\|^2_{-1} \right). \tag{1.53}$$

Here we use the notation $\mathbf{v} = \mathbf{v}(\rho)$ to indicate that the mechanical equilibrium (1.40) determines the deformation field $\mathbf{v}$ for given concentration ρ. For the time-discrete Cahn-Hilliard model we therefore get the energy decay

$$\begin{aligned} &\mathbf{E}^\varepsilon_{\mathbf{pf}}(\rho_{\Delta t}, \mathbf{u}_{\Delta t})(t) + \frac{1}{2}\int_0^t \|\nabla w_{\Delta t}\|^2_{L^2(\Omega)} \\ &= \int_\Omega \left(\tfrac{\varepsilon}{2}|\nabla \rho_{\Delta t}(t)|^2 + \tfrac{1}{\varepsilon}\Psi(\rho_{\Delta t}(t)) + W(\rho_{\Delta t}(t), \mathcal{E}(\mathbf{u}_{\Delta t}(t)))\right) + \tfrac{1}{2}\int_0^t \|\nabla w_{\Delta t}\|^2_{L^2(\Omega)} \le \mathbf{E}_0 \end{aligned} \tag{1.54}$$

for $t \in [m\,\delta t, (m+1)\delta t]$, which follows from (1.37). Here we extend the time-discrete functions by setting them piecewise constant, for instance $\rho_{\Delta t}(t) := \rho^i$ for $t \in [i\Delta t, (i+1)\Delta t)$ and $\mathbf{E}_0$ is the given energy at initial time $t = 0$. The replacement of the time difference quotient $\frac{1}{\Delta t}\|\rho^i - \rho^{i-1}\|_{-1}$ by $\|\nabla w\|_{L^2(\Omega)}$ is according to (1.51).

As it has been shown in [Gar00] – in an even more general setting –, there exists a minimiser for sufficiently small time steps Δt. The main point is to show coerciveness of the energy functional, not regarding the $\|.\|_{-1,2}$-Norm, but the $H^{1,2}$-Norm.

Remark. Another way to motivate the resulting phase-field equations from the energy functional $\mathbf{E}^\varepsilon_{\mathbf{pf}}$ is to take $\frac{\delta \mathbf{E}^\varepsilon_{\mathbf{pf}}}{\delta \rho} =: w^\varepsilon$ as a potential which induces a mass flow $J = -\nabla w^\varepsilon$. Balance of mass then leads to the equation

$$\partial_t \rho^\varepsilon = -\nabla \cdot J = \Delta w^\varepsilon.$$

See [Gar00] and [Gar03] for more details.

Remark. The sharp-interface Mullins-Sekerka model can also be described formally as a gradient flow in an appropriate setting. This derivation has been done in [GLNRW06].

1.4 Weak formulation of phase-field solution

From the above time-discrete ansatz we can get a weak solution of the phase-field equations (1.40) and (1.41) by passing to the limit $\Delta t \to 0$. To be precise we have

Proposition 1.3. *For initial concentration value ρ^0 the time-discrete functions derived in the above section converge along a sequence $\Delta t \to 0$ to limit functions $\rho^\varepsilon \in L^2(0,T;\mathcal{M}) \cap H^{1,2}(0,T;\mathcal{M}^*)$, $w^\varepsilon \in L^2(0,T;H^{1,2}(\Omega))$ and $\mathbf{u}^\varepsilon \in L^2(0,T;H^{1,2}(\Omega,\mathbb{R}^d))$ in the following way*

$$\varrho_{\Delta t} \to \rho^\varepsilon \qquad \text{in } L^\infty(0,T;L^2(\Omega)), \text{ and weak-}* \text{ in } L^\infty(0,T;H^{1,2}(\Omega)) \tag{1.55}$$

$$\bar{\varrho}_{\Delta t} \to \rho^\varepsilon \qquad \text{in } C^{0,\alpha}(0,T;L^2(\Omega)) \text{ for some } \alpha > 0, \tag{1.56}$$

$$\mathbf{v}_{\Delta t} \to \mathbf{u}^\varepsilon \qquad \text{in } L^2(0,T;H^{1,2}(\Omega,\mathbb{R}^d)), \tag{1.57}$$

$$w_{\Delta t} \rightharpoonup w^\varepsilon \qquad \text{weakly in } L^2(0,T;H^{1,2}(\Omega)), \tag{1.58}$$

$$\Psi'(\varrho_{\Delta t}) \to \Psi'(\rho^\varepsilon) \qquad \text{in } L^1((0,T)\times\Omega). \tag{1.59}$$

Here $\bar{\varrho}$ is the (in time) piecewise linearly interpolated extension of $(\rho^i)_i$ from the time-discretisation. Furthermore the functions $(\rho^\varepsilon, w^\varepsilon, \mathbf{u}^\varepsilon)$ form a weak solution of (1.40) *and* (1.41) *in the following sense*

$$-\int_{(0,T)\times\Omega} \partial_t \xi \cdot (\rho^\varepsilon - \rho^0) + \int_{(0,T)\times\Omega} \nabla w^\varepsilon \cdot \nabla \xi = 0, \tag{1.60}$$

for all $\xi \in L^2(0,T;H^{1,2}(\Omega))$ with $\partial_t \xi \in L^2((0,T)\times\Omega)$ and $\xi(T) = 0$,

$$\int_{(0,T)\times\Omega} w^\varepsilon \zeta = \int_{(0,T)\times\Omega} \tfrac{\varepsilon}{2} \nabla \rho^\varepsilon \cdot \nabla \zeta + \tfrac{1}{\varepsilon} \Psi'(\rho^\varepsilon)\zeta + W_{,\rho}(\rho^\varepsilon, \mathcal{E}(\mathbf{u}^\varepsilon))\zeta, \tag{1.61}$$

for all $\zeta \in L^2(0,T;H^{1,2}(\Omega)) \cap L^\infty((0,T)\times\Omega)$ and

$$\int_{(0,T)\times\Omega} W_{,\mathcal{E}}(\rho^\varepsilon, \mathcal{E}(\mathbf{u}^\varepsilon)) : (D\eta) = 0 \tag{1.62}$$

for all $\eta \in L^2(0,T;H^{1,2}(\Omega,\mathbb{R}^d))$.

Proof. The existence of the time-discrete functions and the above convergences to a weak solution of the Cahn-Larché system has been shown in [Gar00] and [Gar03]. □

Remark.

- In Subsection 1.3 the natural space of test-functions was $L^2(0,T;H_0^{1,2}(\Omega))$. But by the discussion about extending functionals on $H^{1,2}(\Omega)$ by setting them zero for constant functions, see (1.46), the above notation is well-posed.
- By the time-discrete ansatz we have for arbitrary initial data with finite energy $\mathbf{E}^\varepsilon_{\mathbf{pf}}(\rho^0, \mathcal{E}(\mathbf{u}^0)) < \infty$ a phase-field solution of the Cahn-Larché equations which has a weak gradient flow structure. We will observe the behaviour of these functions in the asymptotic analysis in Chapter 3.

Note that due to the quasi-stationary behaviour of the mechanical forces one actually does not need to specify the initial data for $\mathbf{u}$. In fact, $\mathbf{u}^0$ is implicitly defined by (1.40) through the initial concentration ρ^0.

Lemma 1.4. *For all $\varepsilon > 0$ and almost all $0 < t < T$ the energy function satisfies*

$$\mathbf{E}^{\varepsilon}_{\mathbf{pf}}(t) + 1/2 \int_0^t \int_\Omega |\nabla w^\varepsilon|^2 \leq \mathbf{E}^{\varepsilon}_{\mathbf{pf}}(0) = \mathbf{E}_0 \tag{1.63}$$

where $\mathbf{E}^{\varepsilon}_{\mathbf{pf}}(t) := \mathbf{E}^{\varepsilon}_{\mathbf{pf}}(\rho^\varepsilon(t,.), \mathbf{u}^\varepsilon(t,.))$ with the limit functions $(\rho^\varepsilon, \mathbf{u}^\varepsilon)$ from Proposition 1.3.

Proof. We have to show that the convergences of the time-discrete functions according to Proposition 1.3 conserve the energy functional estimate (1.54). By Proposition 1.3 we have the strong convergence of the concentration function in $L^\infty(0,T; L^2(\Omega))$. Then for a subsequence $(\Delta t)_k \to 0$

$$\rho_{(\Delta t)_k}(t,.) \to \rho^\varepsilon(t,.) \qquad \text{in } L^2(\Omega) \tag{1.64}$$

for almost every $t \in [0,T]$. Then a subsequence of $(\Delta t)_k$ which we again denote by $(\Delta t)_k \to 0$ the functions converge pointwise for almost every $x \in \Omega$

$$\rho_{(\Delta t)_k}(t,.) \to \rho^\varepsilon(t,.) \qquad \text{for almost all } x \in \Omega.$$

At the same time we have by the weak-* convergence for almost every $t \in [0,T]$ the upper bound

$$\|\rho_{(\Delta t)_k}(t,.)\|_{H^{1,2}(\Omega)} < C. \tag{1.65}$$

Then for a subsequence $(\Delta t)_{k'}$, which might depend on $t \in [0,T]$, we have a weakly converging sequence to some $\varrho \in H^{1,2}(\Omega)$

$$\rho_{(\Delta t)_{k'}}(t,.) \rightharpoonup \varrho(.) \qquad \text{in } H^{1,2}(\Omega). \tag{1.66}$$

Using the compact embedding $H^{1,2}(\Omega) \hookrightarrow L^p(\Omega)$ we get

$$\rho_{(\Delta t)_{k'}}(t,.) \to \varrho(.) \qquad \text{in } L^p(\Omega). \tag{1.67}$$

Since for every converging subsequence $(\Delta t)_{k'}$ we can compare the limit function ϱ with the one from (1.64), the two limit functions must coincide $\varrho(.) = \rho^\varepsilon(t,.)$. Moreover the whole sequence $\rho_{(\Delta t)_k}(t,.)$ converges weakly in $H^{1,2}(\Omega)$ for almost every $t \in [0,T]$ to $\rho^\varepsilon(t,.)$. Thus we can conclude

$$\liminf_{(\Delta t)_k \to 0} \int_\Omega |\nabla \rho_{(\Delta t)_k}(t,.)|^2 \geq \int_\Omega |\nabla \rho^\varepsilon(t,.)|^2 \tag{1.68}$$

by the weakly lower semi-continuity of the norm.

The potential Ψ is not convex, so it won't be weakly lower semi-continuous. Together with the estimate

$$|\Psi(r)| \leq C(|r|^p + 1)$$

-which follows from (1.10)- and the convergence in (1.67), we have that $\Psi(\rho_{(\Delta t)_k}(t,.))$ is dominated by a converging sequence of integrable functions for almost every $t \in [0,T]$. Then we can apply Lebesgue's dominated convergence theorem (see for instance Theorem 1.21 in [Alt02]) to get along the chosen subsequence $(\Delta t)_k \to 0$

$$\lim_{(\Delta t)_k \to 0} \int_\Omega \Psi(\rho_{(\Delta t)_k}(t,.)) = \int_\Omega \Psi(\rho^\varepsilon(t,.)). \tag{1.69}$$

The deformation vector converges strongly in $L^2(0,T;H^{1,2}(\Omega))$, so we have with the strong convergence (1.64)

$$\lim_{(\Delta t)_k \to 0} \int_\Omega W(\rho_{(\Delta t)_k}(t,.), \mathbf{u}_{(\Delta t)_k}(t,.)) = \int_\Omega W(\rho^\varepsilon(t,.), \mathbf{u}^\varepsilon(t,.)). \tag{1.70}$$

Finally we observe that from the weak convergence of $w_{\Delta t}$ we have the weak lower semi-continuous limit

$$\liminf_{\Delta t \to 0} \int_0^t \int_\Omega |\nabla w_{\Delta t}|^2 \geq \int_0^t \int_\Omega |\nabla w^\varepsilon|^2$$

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

Now we see that for all $t \in [0,T]$ such that the estimates (1.68), (1.69) and (1.70) hold, the energy dissipation inequality also holds for the phase-field solution $(\rho^\varepsilon, \mathbf{u}^\varepsilon)$ from Proposition 1.3:

$$\mathbf{E}^\varepsilon_{\mathbf{pf}}(\rho^\varepsilon(t,.), \mathbf{u}^\varepsilon(t,.)) + 1/2 \int_0^t \int_\Omega |\nabla w^\varepsilon|^2 \leq \mathbf{E}_0.$$

□

Remark. As the system does not remember its history – note that in (1.53) the only information is the present state, see also (1.37) –, the energy decay can be extended to

$$\mathbf{E}^\varepsilon_{\mathbf{pf}}(\rho^\varepsilon(t_2,.), \mathbf{u}^\varepsilon(t_2,.)) + 1/2 \int_{t_1}^{t_2} \int_\Omega |\nabla w^\varepsilon|^2 \leq \mathbf{E}^\varepsilon_{\mathbf{pf}}(\rho^\varepsilon(t_1,.), \mathbf{u}^\varepsilon(t_1,.))$$

for almost every $t_1, t_2 \in [0,T]$. Thus the energy functional $t \mapsto \mathbf{E}^\varepsilon_{\mathbf{pf}}(t)$ is non-negative and monotonically decreasing.

Lemma 1.5.

(i) By the choice of p and d we have $\Psi'(\rho^\varepsilon) \in L^2(\Omega)$.

(ii) $W_{,\rho}(\rho^\varepsilon, \mathbf{u}^\varepsilon) \in L^2(\Omega)$.

Proof. ad (*i*) We have for $d \leq 3$ the Sobolev-embedding $H^{1,2}(\Omega) \hookrightarrow L^6(\Omega)$. Now note that

$$\Psi'(\rho^\varepsilon) \in L^2(\Omega) \iff \rho^\varepsilon \in L^{2(p-1)}(\Omega)$$

which applies for $p \in (2,4]$ and $d \leq 3$.

ad (ii) This follows by the growth bound (1.4) and part (i).

□

One immediate consequence from the above lemma is

Lemma 1.6. *In equation* (1.61) *we can omit the* $L^\infty(\Omega \times [0,T])$*-restriction for the test-function* ζ*, i.e. equation* (1.61) *holds for all* $\zeta \in L^2(0,T;H^{1,2}(\Omega))$.

Remark. In more general cases the L^∞-restriction on the test-functions for (1.61) has to be made, since from the existence result one only has L^1-integrability of Ψ' and $W_{,\rho}$. Our assumptions on p, d and the elastic energy W simplifies our system of phase-field functions. This is also one difference from the work of Chen, [Chen96], who assumes to have smooth enough phase-field functions.

We can conclude for the weak solution higher regularity in the case of homogeneous elasticity. The higher regularity is crucial to partially integrate as in subsection 3.2.5 and to proof Theorem 3.4. To get an estimate of the discrepancy measure a blow-up technique is applied. There elliptic regularity theory in $H^{2,2}(\Omega)$ is extensively used.

Proposition 1.7. *For homogeneous elasticity the concentration function* ρ^ε *and deformation vector* $\mathbf{u}^\varepsilon$ *are in fact in* $L^2(0,T;H^{2,2}(\Omega))$ *and* $L^2(0,T;H^{2,2}(\Omega,\mathbb{R}^d))$ *respectively.*

Proof. In the case that W is of the quadratic form (1.2) with constant elasticity tensor $\mathcal{C}$, i.e. in the homogeneous case, the equation (1.40) can be re-arranged so that the concentration and deformation field are separated:

$$\operatorname{div} S = \operatorname{div}[\mathcal{C}(\mathcal{E}(\mathbf{u}^\varepsilon) - \mathcal{E}^*(\rho^\varepsilon))] = 0 \quad \Longleftrightarrow \quad \operatorname{div}[\mathcal{C}\mathcal{E}(\mathbf{u}^\varepsilon)] = \operatorname{div}[\mathcal{C}\mathcal{E}^*(\rho^\varepsilon)].$$

This is in fact an elliptic system with constant coefficients for $\mathbf{u}^\varepsilon$ by the properties of $\mathcal{C}$. As ρ^ε is in $H^{1,2}(\Omega)$, the right-hand side is in $L^2(\Omega)$ and therefore $\mathbf{u}^\varepsilon$ is in $H^{2,2}(\Omega)$ by elliptic regularity theory.

Then again we look back at equation (1.13) which is an elliptic equation for ρ^ε, a Poisson equation with a right side in $L^2(\Omega)$:

$$\Delta\rho^\varepsilon = \frac{1}{\varepsilon}\left(\frac{1}{\varepsilon}\Psi'(\rho^\varepsilon) + W_{,\rho}(\rho^\varepsilon, \mathcal{E}(\mathbf{u}^\varepsilon)) - w^\varepsilon\right).$$

By elliptic regularity theory ρ^ε is also in $H^{2,2}(\Omega)$. This holds for almost every time t and by the continuity of above arguments the claim of our proposition holds. □

1.4.1 Pointwise in time equations

The equations (1.60) to (1.62) have analogue equations for almost every time t. This is probably more common to most readers. We will use these pointwise in time equations in Subsections 3.2.5 and 3.2.8.

First, we use partial integration in equation (1.60) to get

$$\int_{(0,T)} \langle \partial_t \rho^\varepsilon, \xi \rangle_{H^{1,2}(\Omega)} ds + \int_{(0,T)\times\Omega} \nabla w \cdot \nabla \xi \, dx \, ds = 0. \tag{1.71}$$

Here we denote by $\langle ., . \rangle_{H^{1,2}(\Omega)}$ the duality pairing $(H^{1,2}(\Omega))^* \times H^{1,2}(\Omega) \to \mathbb{R}$. Note that now the equations (1.71), (1.61) and (1.62) do not involve any time derivatives of the test function.

Now we choose test-functions for $0 \leq t_1 < t_2 \leq T$ of the following form:

$$\xi(x,t) := \frac{\chi_{[t_1,t_2]}(t)}{t_2 - t_1} \hat{\xi}(x), \quad \zeta(x,t) := \frac{\chi_{[t_1,t_2]}(t)}{t_2 - t_1} \hat{\zeta}(x), \quad \eta(x,t) := \frac{\chi_{[t_1,t_2]}(t)}{t_2 - t_1} \hat{\eta}(x), \tag{1.72}$$

where $\hat{\xi}, \hat{\zeta} \in H^{1,2}(\Omega)$ and $\hat{\eta}(x) \in H^{1,2}(\Omega, \mathbb{R}^d)$.

Sending $(t_2 - t_1) \to 0$ we get for almost all $t \in [0, T]$

$$\langle \partial_t \rho^\varepsilon, \hat{\xi} \rangle_{H^{1,2}(\Omega)} + \int_\Omega \nabla w \cdot \nabla \hat{\xi} = 0, \tag{1.73}$$

$$\int_\Omega w^\varepsilon \hat{\zeta} = \int_\Omega \tfrac{\varepsilon}{2} \nabla \rho^\varepsilon \cdot \nabla \hat{\zeta} + \Psi'(\rho^\varepsilon) \hat{\zeta} + W_{,\rho}(\rho^\varepsilon, \mathcal{E}(\mathbf{u}^\varepsilon)) \hat{\zeta}, \tag{1.74}$$

$$\int_\Omega W_{,\mathcal{E}} : D(\hat{\eta}) = 0. \tag{1.75}$$

Note that the times $t \in [0, T]$ for which above equations hold correspond in fact to the Lebesgue-points of (1.71), (1.61) and (1.62) in the time interval $[0, T]$.

Inhomogeneous elasticity

Initially we tried to incorporate inhomogeneous elasticity with $\mathcal{C} = \mathcal{C}(\rho)$ as well. Lemma 1.5 and Proposition 1.7 would need an adaption or replacement. Especially the techniques in Subsection 3.2.8 don't seem to be adaptable.

We will derive the a priori estimates

$$\|\rho^\varepsilon\|_{H^{1,1}(\Omega)} + \|\mathbf{u}^\varepsilon\|_{H^{1,2}(\Omega)} < C,$$

which we use for compactness. In the inhomogeneous elasticity case

$$W(\rho, \mathcal{E}) = \tfrac{1}{2}\big(\mathcal{E} - \mathcal{E}^*(\rho)\big) : \mathcal{C}(\rho)\big(\mathcal{E} - \mathcal{E}^*(\rho)\big)$$

we have

$$\operatorname{div} S = 0 \quad \Longleftrightarrow \quad \operatorname{div}[\mathcal{C}\mathcal{E}(\mathbf{u}^\varepsilon)] = \operatorname{div}[\mathcal{C}\mathcal{E}^*(\rho^\varepsilon)],$$

an elliptic system for $\mathbf{u}$, but the coefficients are now merely measurable. Although in dimension 2 they are continuous by the Sobolev embedding theory, with the estimate

$$|W_{,\rho}(\rho^\varepsilon, \mathbf{u}^\varepsilon)| \leq C(1 + |\rho^\varepsilon|^2 + |\mathcal{E}(\mathbf{u}^\varepsilon)|^2)$$

we obtain that $W_{,\rho}$ is still only L^1-integrable with uniform bounds with respect to ε, cf. estimate (1.4) for homogeneous elasticity. But in Subsection 3.2.8 we will need a uniform bound in $L^2(\Omega)$ for $W_{,\rho}$ which effectively requires $\mathbf{u}$ to be uniformly bound in $H^{1,4}(\Omega)$, so the present arguments won't work with inhomogeneous elasticity. See also remarks in Subsection 3.2.9.

2 Geometric Measure Theory

We introduce some notations and recall some facts about measures and varifolds, see [EvGar92], [Fed69] and [Sim83] for more detailed information. We want to motivate how the notion of curvature is generalised by the first variation of a varifold. Additionally we present cases where a varifold reduces to a countably $(d-1)$-rectifiable set together with a density function.

2.1 Measures

First we recall the definition of a Radon measure μ on an open and bounded domain $\Omega \subset \mathbb{R}^d$ as a Borel regular measure that is finite on compact sets. To a measure μ we introduce the notion of $(d-1)$-dimensional densities on Ω for $x \in \bar{\Omega}$

$$\theta^{*d-1}(\mu, x) = \limsup_{\rho \to 0} \frac{\mu(\Omega \cap B_\rho(x))}{\omega_{d-1}\rho^{d-1}},$$
$$\theta_*^{d-1}(\mu, x) = \liminf_{\rho \to 0} \frac{\mu(\Omega \cap B_\rho(x))}{\omega_{d-1}\rho^{d-1}}.$$

Here ω_{d-1} is the volume of the $(d-1)$-dimensional unit ball. If $\theta^{*d-1}(\mu, x)$ and $\theta_*^{d-1}(\mu, x)$ coincide, this common value will be denoted by $\theta^{d-1}(\mu, x)$.

Definition 2.1. A set $M \subset \mathbb{R}^d$ is called *countably* $(d-1)$*-rectifiable*, if there exist a set M_0 with $\mathcal{H}^{d-1}(M_0) = 0$ and Lipschitz functions $F_j \colon \mathbb{R}^{d-1} \to \mathbb{R}^d$ such that

$$M \subset M_0 \cup \bigcup_{j \in \mathbb{N}} F_j(\mathbb{R}^{d-1}).$$

Lemma 2.2. *A set* $M \subset \mathbb{R}^d$ *is countably* $(d-1)$*-rectifiable, if and only if*

$$M \subset \bigcup_{j=0}^{\infty} N_j$$

with $\mathcal{H}^{d-1}(N_0) = 0$ *and* N_j *is a* $(d-1)$*-dimensional embedded* C^1*-submanifold for each* $j \geq 1$.

Proof. This lemma follows from Whitney's extension theorem:

> For all Lipschitz-continuous $f \colon \mathbb{R}^d \to \mathbb{R}$ and for all $\varepsilon > 0$ there exists a $g \in C^1(\mathbb{R}^d)$ such that
>
> $$\mathcal{L}^d(\{f \neq g\} \cup \{\nabla f \neq \nabla g\}) < \varepsilon$$

□

This lemma indicates that one has some smooth C^1-structure on a countably rectifiable set which leads to tangent spaces in an approximative context. This will be specified in the following definition.

Definition 2.3. Let M be a $\mathcal{H}^{d-1}$-measurable subset of $\mathbb{R}^d$ and θ a positive, locally $\mathcal{H}^{d-1}$-integrable function on M. Then we call a $(d-1)$-dimensional subspace $P = T_{x_0}^{\text{app}} M$ of $\mathbb{R}^d$ the *approximate tangent space $T_{x_0}^{app} M$ for M at $x_0 \in M$ with respect to θ*, if

$$\lim_{\lambda \to 0} \lambda^{-(d-1)} \int_M \phi(\lambda^{-1}(z - x_0))\theta(z) d\mathcal{H}^{d-1}(z) = \theta(x_0) \int_P \phi(z) d\mathcal{H}^{d-1}(z) \quad \forall \phi \in C_0^0(\mathbb{R}^d).$$

Remark. This approximate tangent space is unique, if it exists.

Theorem 2.4. *Let M be a $\mathcal{H}^{d-1}$-measurable subset of $\mathbb{R}^d$. Then M is countably $(d-1)$-rectifiable, if and only if there exists a positive, locally $\mathcal{H}^{d-1}$-integrable function θ on M, such that almost $\mathcal{H}^{d-1}$-everywhere there exists the approximate tangent space with respect to θ.*

Theorem 2.5. *Let μ be a Radon measure on $\mathbb{R}^d$ and define for $x \in \mathbb{R}^d, \lambda > 0$*

$$\mu_{x,\lambda}(A) := \lambda^{-(d-1)} \mu(x + \lambda A) \quad \textit{for Borel sets } A \subset \mathbb{R}^d.$$

If for μ-almost all x there exist some $\theta(x) \in (0, \infty)$ and a $(d-1)$-dimensional subspace P such that

$$\lim_{\lambda \to 0} \int_{\mathbb{R}^d} \phi(y) d\mu_{x,\lambda}(y) = \theta(x) \int_P \phi(y) d\mathcal{H}^{d-1}(y), \tag{2.1}$$

then the set

$$M := \{x \mid \textit{there exist some } P \textit{ and } \theta(x) \textit{ such that } (2.1) \textit{ holds}\}$$

is countably $(d-1)$-rectifiable, θ is $\mathcal{H}^{d-1}$-measurable and $\mu = \mathcal{H}^{d-1} \lfloor_M \lfloor_\theta$, where we set $\theta(x) = 0$ for all $x \notin M$.

Remark. Here $\Omega = \mathbb{R}^d$ is chosen, so that for the rescaling of the measure μ one does not have to worry about rescaling the underlying set as well. Of course, any measure on some subset Ω can be extended by zero on all $\mathbb{R}^d$.

Proof. See [Sim83]. □

2.2 Varifolds

The initial motivation to introduce the concept of varifolds came from the famous geometric *Plateau problem: which surface has the smallest area with a given boundary?* A short introduction and overview to the connection between the theory of minimal surfaces and geometric measure theory can be found in [Alm01].

We look on above mentioned countably $(d-1)$-rectifiable pairs (M, θ) and introduce the equivalence relation

$$(M, \theta) \sim (\tilde{M}, \tilde{\theta}) \quad \Longleftrightarrow \quad \begin{cases} \mathcal{H}^{d-1}((M \setminus \tilde{M}) \cup (\tilde{M} \setminus M)) = 0, \\ \theta(x) = \tilde{\theta}(x) \quad \text{for } \mathcal{H}^{d-1} - \text{a.e. } x \in \mathbb{R}^d. \end{cases} \tag{2.2}$$

Definition 2.6. For a countably $(d-1)$-rectifiable pair (M,θ) we call the equivalence class $V = V(M,\theta)$ by the relation (2.2) a *rectifiable* $(d-1)$*-varifold* (or shortly *rectifiable varifold,* since in our case we don't work with other varifolds than $(d-1)$-varifolds). θ is called the *multiplicity function* of V. If θ has only integer values, we call V an *integral* $(d-1)$*-varifold* or short *integral varifold.*

(i) Associated to a rectifiable varifold V there is a Radon measure μ_V as the *weight measure of* V defined by
$$\mu_V = \mathcal{H}^{d-1}\lfloor_M \lfloor_\theta.$$

(ii) The *total mass of* V is the quantity
$$M(V) := \mu_V(\mathbb{R}^d).$$

Remark. By Theorem 2.5 a Radon measure μ is a weight measure of some rectifiable varifold, if and only if it has an approximate tangent space $T_x^{\text{app}}\mu$ with multiplicity $\theta(x)$ for μ-almost every x. Theorem 2.5 also leads to the definition of the tangent space of a varifold.

Definition 2.7. To a rectifiable varifold $V = V(M,\theta)$ we define the tangent space T_xV to be the approximate tangent space $T_x^{\text{app}}\mu_V$ as in Theorem 2.5.

In contrast to a rectifiable varifold the class of general varifold abandons the definition of the tangent space according to the spatial information. Moreover, we look on the set of $(d-1)$-dimensional subspaces
$$\mathbb{P}^{d-1} := \{P \mid P \text{ is a } (d-1)\text{-dimensional subspace in } \mathbb{R}^d\} \cong \mathbb{S}^{d-1}/\{\pm 1\}.$$

We will use the same notation P for the orthogonal projection onto the subspace P. On $\mathbb{P}^{d-1}$ we use the metric induced by endomorphisms:
$$d(P,Q) := \|P-Q\|_{End}.$$

By the metric we have a topology on $\mathbb{P}^{d-1}$ and this enables us to define a general varifold:

Definition 2.8. A general $(d-1)$-*varifold* on $\Omega \subset \mathbb{R}^d$ or short just *varifold* is a Radon measure on the *Grassmanian manifold*
$$G(\bar{\Omega}) := \bar{\Omega} \times \mathbb{P}^{d-1}. \tag{2.3}$$

(i) Associated to a varifold we have the *mass measure* μ_V of a varifold given by
$$\mu_V(A) := V(\pi^{-1}(A)) = \int_{A\times\mathbb{P}^{d-1}} dV(x,P) \quad \text{for } A \subset \bar{\Omega}$$

where π is the projection onto the spatial part: $\pi\colon \bar{\Omega}\times\mathbb{P}^{d-1} \to \bar{\Omega},\ (x,P) \mapsto x.$

(ii) The *total mass* of a varifold is defined by

$$M_V := \mu_V(\bar{\Omega}).$$

Remark. If $V = V(M, \theta)$ is a rectifiable varifold, then it can be seen as a general varifold in the following way:

Set $M^* := \{x \in M \mid M \text{ has approx. tangent space } T_x^{\text{app}} M\}$, $TM := \{(x, T_x^{\text{app}} M) \mid x \in M^*\}$ and $\mu := \mathcal{H}^{d-1}\lfloor_M \lfloor_\theta$. Then

$$V(\mathcal{A}) = \mu(\pi(TM \cap \mathcal{A})), \quad \forall \mathcal{A} \subset G(\Omega).$$

The measure μ coincides with the mass measure μ_V of this varifold.

Remark.

- We use such varifolds to describe interfaces. Since varifolds are defined simply as Radon measures on $\bar{\Omega} \times \mathbb{P}^{d-1}$, the tangential information is given independently of the spatial information (of a neighbourhood). In this sense the actual information of a varifold is a-priori very vague.

- For a C^1-hypersurface $\mathfrak{M}$, we can introduce a corresponding varifold $V_{\mathfrak{M}}$ by setting
$$dV_{\mathfrak{M}}(x, P) = d\mathcal{H}^{d-1}\lfloor_{\mathfrak{M}}(x)\, \delta_{T_x\mathfrak{M}}(P).$$
We denote by $\delta_{T_x\mathfrak{M}}$ the Dirac measure concentrated on $T_x\mathfrak{M}$.

The motivation to use varifolds is that the limit interface will not provide sufficient smoothness to fulfil some kind of Gibbs-Thomson law in the classical sharp interface sense. In fact Schätzle has shown in [Sch97] that even the BV-formulation of the Gibbs-Thomson law breaks down when two interfaces touch each other. He introduced the notion of varifolds to come up with a formulation which extends the model beyond the time of topological changes.

Through the notion of varifolds we are able to describe so-called *phantom interfaces*, which are not captured by characteristic functions. Figure 4 gives an illustration of a time-independent example. Assume that the two regions of approximations χ^ε merge to one when letting $\varepsilon \to 0$. Then the dashed line is a phantom interface.

Bronsard and Stoth studied the related Allen-Cahn equation and proved that in the limit there exist interfaces with arbitrary high multiplicity, see [BroSto96].

2.2.1 First Variation of a varifold

In the smooth classical sense the Gibbs-Thomson law incorporates the mean curvature κ. Actually the curvature term occurs through the first variation of the area. For varifolds one has to use the first variation formula derived in Allard [All72] and Simon [Sim83].

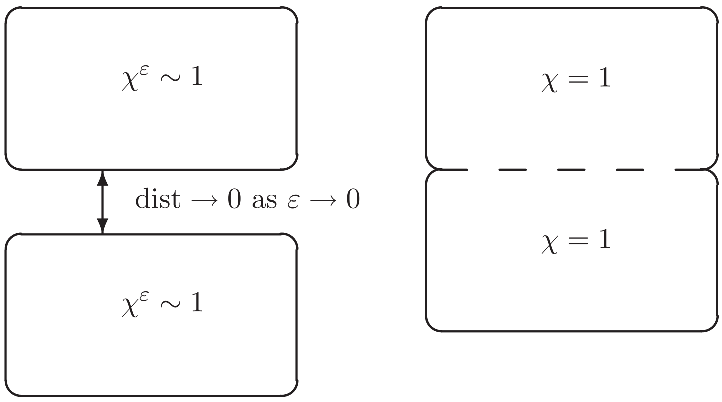

Figure 4: An example where phase-field interfaces lead to a phantom interface in the limit $\varepsilon \to 0$.

As it can be found in the aforementioned works of Allard and Simon, the first variation of a varifold is given by

$$\delta V(X) = \int_{G(\Omega)} DX(x) : P \, dV(x, P) \quad \text{for } X \in C_0^1(\Omega, \mathbb{R}^d) \tag{2.4}$$

where $DX(x) : P$ is defined to be the inner product between linear mappings and $DX(x) : P$ is in fact the divergence of X with respect to the linear subspace P.

In fact, this coincides with the mean curvature in the smooth case. Using the Gauss theorem on a C^2-hypersurface $\mathfrak{M}$

$$\int_{\mathfrak{M}} \operatorname{div}_{\mathfrak{M}} X \, d\mathcal{H}^{d-1} = \int_{\mathfrak{M}} X \cdot \nu_{\mathfrak{M}} \kappa_{\mathfrak{M}} \, d\mathcal{H}^{d-1}$$

with an arbitrary unit normal $\nu_{\mathfrak{M}}$ to $\mathfrak{M}$ and $\kappa_{\mathfrak{M}}$ the scalar mean curvature of $\mathfrak{M}$ with the sign according to $\nu_{\mathfrak{M}}$, if $\mathfrak{M}$ does not have any boundary part in the support of X. One notices that for $X \in C_0^1(\Omega, \mathbb{R}^d)$ the variation of the area can thus be read as the surface divergence of the vector field, i.e. the full divergence minus the normal part of DX.

In the case that the varifold is less smooth, but still has locally bounded first variation, one gets the following decomposition:

If $\|\delta V\|$ is a Radon measure, i.e. a locally bounded measure meaning

$$\forall K \subset\subset \Omega \quad \exists c_K > 0\colon \quad |\delta V(X)| < c_K \|X\|_\infty \quad \forall X \in C_0^1(K, \mathbb{R}^d),$$

the first variation of V can be extended to a bounded operator on $C^0(\Omega, \mathbb{R}^d)$ and one has a $\|\delta V\|$-measurable function $\nu\colon \Omega \to \mathbb{P}^{d-1}$ such that

$$\delta V(X) = \int_\Omega X \cdot \nu \, d\|\delta V\|.$$

We now take the Lebesgue decomposition of $\|\delta V\|$ with respect to μ_V:

$$\delta V(X) = \int_\Omega X \cdot \nu \, d\|\delta V\| = \int_\Omega X \cdot \vec{H}_V \, d\mu_V + \int_Z X \cdot \nu \, d\sigma \tag{2.5}$$

where $\vec{H}_V$ is the Radon-Nikodym derivative of $\|\delta V\|$ with respect to μ_V multiplied with the normal function ν:

$$\vec{H}_V(x) = \nu(x) D_{\mu_V} \|\delta V\|(x).$$

$\vec{H}_V$ is called *generalised mean curvature vector*. The set of singularities $Z := \{x \in \mathbb{R}^d \mid D_{\mu_V}\|\delta V\|(x) = \infty\}$ is the *generalised boundary* of V with *generalised boundary measure* σ, *generalised unit co-normal* $\nu|_Z$ and $\mu_V(Z) = 0$.

One important property of varifolds, even in the general case, is the compactness: Since the Grassmanian manifold $G(\bar{\Omega})$ is a compact space, the space of Radon measure inherits the weak*-topology from the space of continuous functions on the Grassmanian. This is the content of the following theorem:

Proposition 2.9. *Let $V_i, i \in \mathbb{N}$ be a sequence of $(d-1)$-varifolds with uniform bounds, i.e. there exists a constant $C > 0$ such that*

$$|V_i(A)| \leq C$$

for all Borel sets $A \subset G(\Omega)$, then there exists a $(d-1)$-varifold V_0 such that

$$\lim_{i \to \infty} V_i(A) = V_0(A)$$

holds for all Borel sets $A \subset G(\Omega)$.

Remark. If one studies the limit of hypersurfaces just by representation by measures in Ω, then still a limit as a measure is observable, but there is no information on tangents passing through in this process. This loss of tangential information is overcome when using varifolds, since the limit measure will still keep some information of the tangential part.

2.2.2 Rectifiable varifolds

In certain cases it is possible to conclude that a given varifold is in fact rectifiable. Typically one attains the existence of a varifold only in its general notation. So, we look for criteria, when we can deduce from additional known properties some higher regularity, here rectifiability.

The most fundamental criteria is stated in Allard's theorem, see [All72].

Theorem 2.10 (Allard)**.** *Suppose a varifold V has locally bounded first variation in Ω and $\theta^{d-1}(\mu_V, x) > 0$ for μ_V-a.e. $x \in \Omega$, then V is already a rectifiable varifold. Moreover for a varifold V with locally bounded first variation in Ω the restriction of V onto $\{x \mid \theta^{*d-1}(\mu_V, x) > 0\} \times \mathbb{P}^{d-1}$ is rectifiable.*

We present two prominent examples which have been established within the last few years. The first theorem by Schätzle uses a certain structure of the first variation to assert rectifiability (see [Sch01]):

Theorem 2.11 (Schätzle)**.** *Let W be a varifold in $\Omega \subset \mathbb{R}^d, w \in H^{1,q}(\Omega), d/2 < q < d, F \subset \Omega$ such that the characteristic function χ_F lies in $BV(\Omega)$. Furthermore we assume*

(i) $\delta W(\eta) = \int_\Omega \operatorname{div}(w\eta)\chi_F \quad \forall \eta \in C_0^1(\Omega, \mathbb{R}^d)$,

(ii) $|\nabla \chi_F| \leq \mu_W$ *and*

(iii) $\|w\|_{H^{1,q}(\Omega)} + \mu_W(\Omega) \leq \Lambda$ *for some* $\Lambda \in \mathbb{R}$.

Then W has locally bounded first variation satisfying

$$\|\vec{H}_W\|_{L^s(\mu_W \lfloor_{B_r(x)})} \leq C_{d,q}(r)\Lambda^{1+1/s} \qquad \forall B_{2r}(x) \subset \Omega,$$

where $s \in \mathbb{R}$ such that $\frac{d-1}{s} = \frac{d}{q} - 1$.

Moreover, W is rectifiable on the set $\{x \in \Omega \mid \theta^{*d-1}(\mu_W, x) > 0\}$.

The main part of the proof is to show a particular monotonicity formula for the density of the mass measure:

Lemma 2.12 (Monotonicity Formula)**.** *For a varifold W which fulfils the assumptions of Theorem 2.11 the function*

$$r \mapsto r^{-(d-1)}\mu_W(B_r(x_0)) + C_{d,q}\min(1, \mathbf{d})^{-1}\Lambda\rho^\alpha \quad \forall x_0 \in \Omega, 0 < r < \mathbf{d}$$

is non-decreasing for $\alpha = 1 - \frac{d-1}{s} \in (0,1)$ with $\mathbf{d} = \operatorname{dist}(x_0, \partial\Omega)$.

Once this monotonicity formula is established, one can use the following theorem by Ziemer:

Theorem 2.13 (Ziemer)**.** *Let μ be a Radon measure on $\mathbb{R}^d$. Then the following statements are equivalent:*

(i) $\mathcal{H}^{d-1}(A) = 0$ *implies that* $\mu(A) = 0$ *for all Borel sets* $A \subset \mathbb{R}^d$ *and there is a constant* $\bar{C}$ *such that* $\left|\int \phi d\mu\right| \leq \bar{C}\|\phi\|_{BV(\mathbb{R}^d)}$ *for all* $\phi \in BV(\mathbb{R}^d)$.

(ii) There is a constant $\bar{C}$ such that $\mu(B_r(x)) \leq \bar{C}r^{d-1}$.

By the theorem of Ziemer we obtain from Lemma 2.12 local bounds for the measure μ_W, i.e. for all $\phi \in BV(\Omega)$ and $B_r(x) \subset \Omega$

$$\left|\int_\Omega \phi\, \chi_{B_r(x)} d\mu_W\right| \leq \bar{C}\|\phi\|_{BV(\mathbb{R}^d)}.$$

Now, we choose $\phi = |w|^s$, which is in $H^{1,1}(\Omega)$ by embedding theorems, and the first variation of the varifold W can therefore be estimated by

$$|\delta W(\eta)| \le \left| \int (w\eta) d\mu_W \right| \le \|w\|_{L^s(\mu_W)} \|\eta\|_{L^{s^*}(\mu_W)}.$$

The second result is by Luckhaus, see [Luck07]. This result applies for weaker assumptions, see Subsection 3.2.9 for an application.

Theorem 2.14 (Luckhaus)**.** *Let W be a $(d-1)$-dimensional varifold on a domain $\Omega \subset \mathbb{R}^d$ whose first variation is given by*

$$\langle \delta W, \phi \rangle = \int_\Omega (v\phi + A : \nabla\phi) d\mu_1, \qquad \phi \in C_0^1(\Omega, \mathbb{R}^d),$$

where the estimate

$$\begin{aligned} r^{-d} \int_{B_r(x)} |A(y)| d\mu_1(y) + r^{-(d-1)} \int_{B_r(x)} |v(y)| d\mu_1(y) & \\ \le \partial_r F \left(r, \sup_{r<R<\operatorname{dist}(x,\partial\Omega)} R^{-(d-1)} \int_{B_R(x)} d\mu_2 \right) & \qquad (2.6) \end{aligned}$$

holds for all $B_r(x) \subset \Omega$ with μ_1, μ_2 non-negative Radon measures on Ω and $F\colon R_{\ge 0} \times R_{\ge 0} \to [0, \infty)$ satisfies

(i) $F(0, L) = 0,\ \partial_r F(r, L) \ge 0,\ \partial_r^2 F(r, L) \le 0$ *for* $r, L \ge 0$,

(ii) $\lim_{L\to\infty} L^{-1} g(L) = 0$ *where* $g(L) := \inf\{R^{1-d} + F(R, L) \mid R > 0\}$.

Moreover assume that

$$\limsup_{r\to 0} r^{1-d} \int_{B_r(x)} d\mu_W \ge \theta > 0$$

for μ_W-almost all $x \in \Omega$. Then W is rectifiable.

More precisely Luckhaus recovers for any $M > 0$ and $\hat{\Omega} \subset\subset \Omega$ an exceptional set $K_M \subset \hat{\Omega}$ with vanishing $\mathcal{H}^{d-1}$-measure for $M \to \infty$, such that for $y_1, y_2 \notin K_M$ the respective values of the projections $P(y_1), P(y_2)$ onto the tangent planes at y_1, y_2 fulfil

$$|P(y_1) - P(y_2)| \le M \left| \ln |y_1 - y_2| \right|^{-1/4}.$$

Comparing this result with theorems 2.4 or 2.5 gives indeed the rectifiability.

3 Asymptotic limit

3.1 Assumptions

We summarise the results of the first chapter about the phase-field system and use them as our starting point of the asymptotic limit. The goal is to observe the behaviour of the functions in the limit $\varepsilon \to 0$. Of special interest is the Gibbs-Thomson law which appears in (1.21) in the phase-field model and will be formulated in a varifold notation, see Definition 3.1 (ii).

Let $\Omega \subset \mathbb{R}^d$ be an open, bounded set with C^2-boundary, $d = 1, 2, 3$. We are further given $m_0 \in (-1, 1)$ and initial data

$$(\rho_0^\varepsilon, \mathbf{u}_0^\varepsilon) \in \{(\rho, \mathbf{u}) \in \mathcal{M}_{m_0} \times \widetilde{\mathcal{M}} \mid \mathbf{E}_{\mathbf{pf}}^\varepsilon(\rho, \mathbf{u}) \leq \mathbf{E}_0\} \tag{$\mathbf{I}$ 1}$$

for $\varepsilon > 0$ where $\mathbf{E}_0$ is a given, positive constant. Here $\mathbf{u}_0^\varepsilon$ is in fact implicitly defined by ρ_0^ε by the quasi-stationary mechanical equilibrium (1.40), see remark after Proposition 1.3. For $\varepsilon \in (0, 1)$ we have weak solutions of the Cahn-Larché system (1.12)-(1.14) of the following form

- $\rho^\varepsilon \in L^2(0, T; H^{2,2}(\Omega)) \cap H^{1,2}(0, T; H^{-1,2}(\Omega)) \cap \{\varrho \mid \int_\Omega \varrho = m_0|\Omega|\}$ with $\rho^\varepsilon|_{t=0} = \rho_0^\varepsilon$,
- $w^\varepsilon \in L^2(0, T; H^{1,2}(\Omega))$,
- $\mathbf{u}^\varepsilon \in L^2(0, T; H^{2,2}(\Omega, \mathbb{R}^d))$

for a $m_0 \in (-1, 1)$, such that the following weak formulation is fulfilled

$$\int_0^T \langle \partial_t \rho^\varepsilon, \zeta_1 \rangle_{H^{1,2}(\Omega)} dt + \int_0^T \int_\Omega \nabla w^\varepsilon \cdot \nabla \zeta_1 \, dx dt = 0, \tag{3.1}$$

$$\int_0^T \int_\Omega w^\varepsilon \zeta_2 \, dx dt = \int_0^T \int_\Omega \varepsilon \nabla \rho^\varepsilon \cdot \nabla \zeta_2 + \tfrac{1}{\varepsilon} \Psi'(\rho^\varepsilon) \zeta_2 + W_{,\rho}(\rho^\varepsilon, \mathcal{E}(\mathbf{u}^\varepsilon)) \zeta_2 \, dx dt, \tag{3.2}$$

$$0 = \int_0^T \int_\Omega S : D\zeta_3 \, dx dt = \int_0^T \int_\Omega W_{,\mathcal{E}}(\rho^\varepsilon, \mathcal{E}(\mathbf{u}^\varepsilon))) : D\zeta_3 \, dx dt \tag{3.3}$$

for all $\zeta_1 \in L^2(0, T; H^{1,2}(\Omega))$, $\zeta_2 \in L^2(0, T; H^{1,2}(\Omega))$ and $\zeta_3 \in L^2(0, T; H^{1,2}(\Omega, \mathbb{R}^d))$. Here, $\langle ., . \rangle_{H^{1,2}(\Omega)}$ is the duality pairing between $H^{-1,2}(\Omega)$ and $H^{1,2}(\Omega)$. As discussed in Sections 1.3 and 1.4 we take $H^{-1,2}(\Omega)$ as the dual space of $H_0^{1,2}(\Omega)$, cf. (1.45).

Remark. By choosing $\mathcal{M} = \mathcal{M}(m_0)$ we have set the mass of the initial concentration independent of ε, i.e. there exists a constant $m_0 \in (-1, 1)$ such that $\int_\Omega \rho_0^\varepsilon = m_0|\Omega|$.

3.1.1 Notes on the asymptotic limit $\varepsilon \to 0$

One important first observation for the limit process $\varepsilon \to 0$ is to identify

$$e^\varepsilon(\rho^\varepsilon) := \tfrac{\varepsilon}{2} |\nabla \rho^\varepsilon|^2 + \tfrac{1}{\varepsilon} \Psi(\rho^\varepsilon) \tag{3.4}$$

as the *interfacial energy density* in the phase-field model. Heuristically, this is the quantity one observes to carry the interfacial energy of the phase-field model, see [MoMo77] for the standard, non-elastic Cahn-Hilliard case and [JLL98] for the Cahn-Larché system. The goal is to show convergence of the interfacial energy to a quantity that will be understood up to a factor as the $\mathcal{H}^{d-1}$-measure of the interface.

Another important function is the so-called *discrepancy measure*

$$\xi^\varepsilon(\rho^\varepsilon) := \tfrac{\varepsilon}{2}|\nabla\rho^\varepsilon|^2 - \tfrac{1}{\varepsilon}\Psi(\rho^\varepsilon). \tag{3.5}$$

As it is stated in Theorem 3.4, in the limit $\varepsilon \to 0$ the discrepancy measure will be non-positive, which means that the Ψ-part is larger than the $|\nabla\rho^\varepsilon|^2$-part. This is essential to verify the varifold structure of the Radon measures we get in Proposition 3.2 (ii).

One consequence of the asymptotic limit which is treated in this chapter is that for the sharp-interface model with given initial data $\Omega_+^0 \subset \Omega$ smooth enough, one has existence of a global in time solution according to below definition. (Note that choosing such a set is a valid initial data, since the other informations are implicitly defined by it - if one neglects possible additional phantom interfaces. This is neglected by demanding Ω_+^0 to be "smooth enough"). One has to choose appropriate initial data ρ_0^ε for the phase-field model, such that

$$\rho_0^\varepsilon \to -1 + 2\chi_{\Omega_+^0} \qquad \text{in } L^2(\Omega).$$

In the formulation of the subsequent propositions and theorems in this chapter the "end time" $T > 0$ is fixed. But by choosing a sequence $T_j \to \infty$ and extending the objects $(M, V, w, \mathbf{u})$ accordingly over time, there are no time bounds as in some other works, see also discussion in Subsection 3.3.

For the evolutionary system we start with a suitable weak formulation of the sharp interface problem (1.19)–(1.22). Through the $\varepsilon \to 0$-limit process one cannot expect that the resulting limit objects are smooth enough such that equations (1.19)–(1.22) can be verified in a classical way. Apart from concentration, the chemical potential and deformation vector which converge quite straightforward in the $\varepsilon \to 0$-limit process, we need for a complete formulation of the Gibbs-Thomson law both a characteristic function and a varifold, which represents the interface as motivated in Subsection 2.2 including possible phantom interfaces.

3.2 Convergence and limit equations

First we specify the notion of a generalised solution of the sharp interface model.

3.2.1 Definition

Definition 3.1 (Generalised solution)**.** $(M, V, w, \mathbf{u})$ is said to be a *generalised solution of the modified Mullins-Sekerka problem*, if

- $M \subset [0,\infty) \times \bar{\Omega}$, $w \in L^2_{\text{loc}}(0,\infty; H^{1,2}(\Omega)), \mathbf{u} \in L^2_{\text{loc}}(0,\infty; H^{1,2}(\Omega,\mathbb{R}^d)),$ V is a Radon measure on $[0,\infty) \times \bar{\Omega} \times \mathbb{P}^{d-1}$.

- Furthermore $\chi_M \in C^0([0,\infty); L^1(\Omega)) \cap L^\infty(0,\infty; BV(\Omega))$ and V^t is a varifold on Ω for all $t > 0$,

such that for all $T > 0$, for almost every $0 < \tau < t < T$ and for all test functions $\zeta \in C_0^1([0,T) \times \bar{\Omega})$, $\vec{Y} \in C_0^1(\Omega, \mathbb{R}^d)$ and $\vec{X} \in L^2(0,T; H^{1,2}(\Omega, \mathbb{R}^d))$ the following holds:

(i) $\int_0^T \int_\Omega [-2\chi_{M^t}\partial_t\zeta + \nabla w \nabla\zeta] = \int_\Omega 2\chi_{M^0}\zeta(0,.)$,

(ii) $2\int_\Omega \chi_{M^t} \operatorname{div}(w\vec{Y}) = \langle \partial V^t, \vec{Y}\rangle + \sum_k \int_{\Omega_k^t} \big(W(k, \mathcal{E}(\mathbf{u}))\,\mathbf{id} - (\nabla\mathbf{u})^T S(k, \mathcal{E}(\mathbf{u}))\big) : D\vec{Y}$,

(iii) $d\mu_{V^t}(x) \geq 2\sigma |D\chi_{M^t}|(x)dx$,

(iv) $\mu_{V^t}(\Omega) + \sum_k \int_{\Omega_k^t} W(k, \mathcal{E}(\mathbf{u})(t,.)) + \int_\tau^t \int_\Omega |\nabla w|^2$
$\leq \mu_{V^\tau}(\Omega) + \sum_k \int_{\Omega_k^\tau} W(k, \mathcal{E}(\mathbf{u})(\tau,.))$,

(v) $\int_0^T \sum_k \int_{\Omega_k^t} S(k, \mathcal{E}(\mathbf{u})) : D\vec{X}\, dxdt = 0$

where the sum over k is taken over $-1, +1$ and $\Omega_k^t := \{x \in \Omega \mid -1 + 2\chi_{M^t}(x) = k\}$ denotes the partition of Ω into its two phases at time t.

Remark. The first equation is the weak formulation of the diffusion equations (1.19) and (1.20). In the bulk the chemical potential will be harmonic. Equation (ii) is the Gibbs-Thomson law (1.21) in a weak formulation (cf. explanations about the first variation of a varifold 2.2.1 and [Gar00]). Equations (ii) and (iii) describe properties of the varifold. Inequality (iii) allows that the varifold can possibly see phantom interfaces. Equation (iv) states the dissipation of the free energy and equation (v) states in a weak form that the stress is divergence free in the bulk, cf. (1.22), and at the same time one obtains that the normal jump of the stress is zero across the interface.

One should notice that the Gibbs-Thomson law has two terms which represent the interface and vanish in the bulk, but the elastic term is still a volume integral. The reason for this is that the elastic energy is a non-local volume energy. So, one has to be aware in the $\varepsilon \to 0$-limit process that both $\frac{\varepsilon}{2}|\nabla\rho^\varepsilon|^2$ and $\Psi(\rho^\varepsilon)$ converge to a $(d-1)$-dimensional measure while the elastic energy W will not vanish in the bulk, thus the support will be generally the whole Ω. See also the remark about Schätzle's result in Subsection 3.3.

If a smooth solution $((\Gamma_t)_{t\geq 0}, w, \mathbf{u})$ with evolving hypersurfaces Γ_t of the sharp interface problem (1.19)-(1.22) is given, then one can easily verify that this also validates as generalised solution. In this case the respective varifold is to be defined as in the remark after Definition 2.8 except for the surface energy constant:

$$dV_{\Gamma_t}^t(x,P) := 2\sigma\, d\mathcal{H}^{d-1}\lfloor_{\Gamma_t}(x)\, \delta_{T_x\Gamma_t}(P). \tag{3.6}$$

3.2.2 Statements

Proposition 3.2. *Let the assumptions mentioned in Section 3.1 hold. Then along a sequence $\varepsilon_i \to 0$ the following holds:*

(i) There exist functions $w \in L^2(0,T;H^{1,2}(\Omega)), \mathbf{u} \in L^2(0,T;H^{1,2}(\Omega,\mathbb{R}^d))$ and a set $M \subset [0,T]\times\Omega$ with $\chi_M \in C^0([0,T];L^1(\Omega)) \cap L^\infty(0,T;BV(\Omega))$ such that

1) $\rho^{\varepsilon_i} \to -1 + 2\chi_M$ in $C^{1/9}([0,T];L^2(\Omega))$ and almost everywhere,

2) $w^{\varepsilon_i} \to w$ weakly in $L^2(0,T;H^{1,2}(\Omega))$,

3) $\mathbf{u}^{\varepsilon_i} \to \mathbf{u}$ in $L^2(0,T;H^{1,2}(\Omega,\mathbb{R}^d))$.

(ii) There exist Radon measures μ, μ_{kl} on $\bar\Omega \times [0,\infty)$ such that

$$e^{\varepsilon_i}(\rho^{\varepsilon_i})dxdt \to d\mu(x,t), \tag{3.7}$$

$$\varepsilon_i(\partial_{x_k}\rho^{\varepsilon_i})(\partial_{x_l}\rho^{\varepsilon_i})dxdt \to d\mu_{kl}(x,t) \tag{3.8}$$

both as Radon measures on $\bar\Omega\times[0,T]$ for all $T>0$.

The varifold is obtained in the following way:

Proposition 3.3. *The measures μ_{kl} from Proposition 3.2 are absolutely continuous with respect to μ, so the Radon-Nikodym derivatives can be represented as functions $\nu_{kl} \in L^1(\mu)$ for $k,l = 1,...,d$. They can be expressed by*

$$\left(\nu_{kl}\right)_{k,l=1}^d = \sum_{i=1}^d \lambda_i \vec\nu_i \otimes \vec\nu_i$$

where $\lambda_i \in [0,1]$, $\sum_i \lambda_i \geq 1$ and $\vec\nu_i$ form an orthonormal basis of $\mathbb{R}^d$. We can use this to define a Radon measure V on $G(\bar\Omega)\times[0,T]$ by

$$dV^t(x,P) = \sum_i \lambda_i(x,t)d\mu(x,t)\delta_{\vec\nu_{i(x,t)}}(P) \qquad \text{for } x \in \bar\Omega, P \in \mathbb{P}^{d-1} \tag{3.9}$$

which is a varifold for almost all times $t \in [0,T]$ and has the following first variation: For all $\vec Y \in C_0^1(\Omega\times[0,T],\mathbb{R}^d)$ it holds

$$\int_0^T \delta V^t(\vec Y) = \int_0^T \int_\Omega \nabla \vec Y : [d\mu(.,t)\,\mathbf{id} - (d\mu_{ij}(.,t))_{ij}]. \tag{3.10}$$

Here we denote by $\delta_{\vec\nu_i}(P)$ the projection onto P, if P is perpendicular to $\vec\nu_i$, and null otherwise. Note that in view of Definition 3.1 (ii) the full description of the Gibbs-Thomson law then is

$$\int_\tau^t \int_\Omega 2\chi_{\Omega_-}\operatorname{div}(w\vec X) = \int_\tau^t \delta V^s(\vec X) + \int_\tau^t \int_\Omega D\vec X : (W\,\mathbf{id} - (\nabla\mathbf{u})^T S). \tag{3.11}$$

In other words, we claim that the term in the brackets in above equation (3.10) is a projection as described in equation (3.9) by the term $\delta_{\vec\nu_i}(P)$, see Subsection 3.2.7 for details.

Remark. To show that the measures μ and μ_{ij} can be used to define a varifold, we need an estimate of the discrepancy measure which is stated in Theorem 3.4.

We define for $\varepsilon > 0$ the set

$$\mathcal{K}_\varepsilon := \{(\rho, v) \in H^{2,2}(\Omega) \times L^2(\Omega) \mid -\varepsilon\Delta\rho + \tfrac{1}{\varepsilon}\Psi'(\rho) = v \text{ in } \Omega \text{ and } \partial_\nu \rho = 0 \text{ on } \partial\Omega\}. \tag{3.12}$$

Theorem 3.4. *There exist a constant $\eta_0 \in (0, 1]$ and continuous and non-increasing functions $M_1(.), M_2(.)\colon (0, \eta_0] \to (0, \infty)$ such that for every $\eta \in (0, \eta_0]$, every $\varepsilon \in (0, M_1(\eta)^{-1}]$ and every $(\rho, v) \in \mathcal{K}_\varepsilon$ it holds*

$$\int_\Omega (\xi^\varepsilon(\rho))^+ \leq \eta \int_\Omega e^\varepsilon(\rho) + \varepsilon M_2(\eta) \int_\Omega v^2. \tag{3.13}$$

Remark. In the application of Theorem 3.4, v will be the difference

$$v = w^\varepsilon - W_{,\rho}(\rho^\varepsilon, \mathcal{E}(\mathbf{u}^\varepsilon)).$$

Finally, we can summarise the above statements and state the main result as

Theorem 3.5. $(M, V, w, \mathbf{u})$ *derived from above theorems form a generalised solution to the modified Mullins-Sekerka problem as defined in Definition 3.1.*

Now that we have stated our results the following subsections are devoted to proofing them. The convergences of Proposition 3.2 are shown subsequently in the next four subsections. At the same time these convergences lead to points (i) and (v) from the definition of a generalised solution 3.1. Additionally the energy functional in the sharp interface case is recovered from the respective phase-field ones, together with the dissipation estimate (iv), see Subsection 3.2.6. In Proposition 3.3 we collect all parts regarding the varifold. In fact to identify a varifold from the measures μ, μ_{ij} the estimate of the discrepancy measure from Theorem 3.4 is necessary. Subsection 3.2.7 shows how the varifold and the weak formulation of the Gibbs-Thomson law (ii) from the definition can be obtained. The extensive proof of Theorem 3.4 is then done in Subsection 3.2.8. It is actually a pointwise in time estimate, but by the uniform bound of the energy and by Corollary 3.14 it is of applicable form for Subsection 3.2.7.

3.2.3 Convergence of concentration

From equations (3.1) and (3.2) one easily gets the following a priori estimates:

Lemma 3.6. *For all $\varepsilon \in (0, 1)$ and almost all $t > 0$ the following holds*

(i) $\frac{1}{|\Omega|} \int_\Omega \rho^\varepsilon(., t) = m_0$,

(ii) $\int_\Omega |\rho^\varepsilon|^p \leq C(1 + \mathbf{E}_0)$,

(iii) $\int_\Omega (|\rho^\varepsilon| - 1)^2 \leq \varepsilon C \mathbf{E}_0$.

Proof.

ad (i) The constant function 1 is an admissible test function in equation (3.1) – see also remark after Proposition 1.3, so the overall mass does not change over time. In the derivation using the gradient flow structure, see Subsection 1.3, we restricted the set of admissible concentration functions to be of a fixed mass. So, in fact this first property is inherited by our model ansatz.

ad (ii) By the convexity of Ψ formulated in (1.10), we have can derive the estimate

$$\Psi(r) \geq C|r|^p - C'.$$

Then we get

$$\int_\Omega |\rho^\varepsilon|^p \leq 2^p C'/C|\Omega| + C^{-1} \int_\Omega \Psi(\rho^\varepsilon) \leq C(1 + \varepsilon \mathbf{E}_0) \leq C(1 + \mathbf{E}_0).$$

ad (iii) Since the function $(|x|-1)^2$ grows with order 2 outside $(-1,1)$ and has exactly two roots, both of order 2, we can find a constant $C > 0$ such that

$$(|x| - 1)^2 \leq C\Psi(x).$$

Here we use the convexity property (1.10) of Ψ. Then we simply have

$$\int_\Omega \left||\rho^\varepsilon| - 1\right|^2 \leq C \int_\Omega \Psi(\rho^\varepsilon) = \varepsilon C \int_\Omega \tfrac{1}{\varepsilon}\Psi(\rho^\varepsilon) \leq \varepsilon C \mathbf{E}_0.$$

□

Remark. The first equation describes one feature of the phase-field model: *conservation of mass* over time. This is essentially due to the diffusion which is driven by a potential and the Neumann boundary conditions.

We now introduce the auxiliary function

$$\tilde{\rho}^\varepsilon(x,t) := \tilde{\rho}^\varepsilon(\rho^\varepsilon(x,t)) := \int_{-1}^{\rho^\varepsilon(x,t)} \sqrt{\tilde{\Psi}(s)/2}ds, \tag{3.14}$$

which is also known as the *Modica ansatz*. Here $\tilde{\Psi}(s) := \min(\Psi(s), 1 + |s|^2)$ is used, so $\tilde{\Psi}$ has the following properties:

Lemma 3.7. *There exist constants $C_1, C_2 > 0$ such that for all $s_1, s_2 \in \mathbb{R}$ the following holds*

$$\int_\Omega |\nabla \tilde{\rho}^\varepsilon(.,t)| = \int_\Omega \sqrt{\tilde{\Psi}(\rho^\varepsilon)/2}\,|\nabla \rho^\varepsilon| \leq \mathbf{E}^\varepsilon_{\mathbf{pf}}(t) \tag{3.15}$$

and

$$C_1|s_1 - s_2|^2 \leq |\tilde{\rho}^\varepsilon(s_1) - \tilde{\rho}^\varepsilon(s_2)| \leq C_2|s_1 - s_2|(1 + |s_1| + |s_2|). \tag{3.16}$$

Proof. (i) The first estimate follows by Young-inequality

$$\int_\Omega \sqrt{\tilde{\Psi}(\rho^\varepsilon)/2}|\nabla\rho^\varepsilon| \le \int_\Omega \tfrac{1}{\varepsilon}\Psi(\rho^\varepsilon) + \tfrac{\varepsilon}{2}|\nabla\rho^\varepsilon|^2 = \int_\Omega e^\varepsilon(\rho^\varepsilon) \le \mathbf{E}^\varepsilon_{\mathbf{pf}}(t)$$

(ii) The inequality on the right is due to

$$|\tilde{\rho}^\varepsilon(s_1) - \tilde{\rho}^\varepsilon(s_2)| \le \left|\int_{s_1}^{s_2} \sqrt{(1+|s|^2)/2}ds\right| \le \left|\int_{s_1}^{s_2} \sqrt{2}(1+|s|)ds\right|.$$

Now, in the last integral the integrand can be estimated by $\sqrt{2}(1+|s|) \le \sqrt{2}(1+|s_1|+|s_2|)$ and the domain of the integral gives the additional factor $|s_1 - s_2|$. The inequality on the left can be deduced by the following:

We want to show that there exists a constant $c_1 > 0$ such that $c_1|s_1 - s_2|^2 \le |\tilde{\rho}^\varepsilon(s_1) - \tilde{\rho}^\varepsilon(s_2)|$ which is equivalent for $s_1 > s_2$ to

$$c_1|s_1 - s_2| \le \frac{\tilde{\rho}^\varepsilon(s_1) - \tilde{\rho}^\varepsilon(s_2)}{s_1 - s_2}.$$

Since the right side is a difference quotient, this holds with some lower bound estimate of the derivative. By definition of $\tilde{\rho}^\varepsilon$ the derivative is

$$\frac{d}{ds}\tilde{\rho}^\varepsilon(s) = \sqrt{\tilde{\Psi}(s)/2}$$

which is strictly positive, moreover $\tilde{\rho}^\varepsilon$ is at least linear (cf. the growth at infinity) with one exception at $s = 1$. This does not cause any problems, since the second derivative is uniformly positive.

□

Using this auxiliary function it is possible to obtain bounds in $BV(\Omega)$.

Lemma 3.8. *For solutions to the Cahn-Larché system the Modica ansatz leads to*

$$\|\tilde{\rho}^\varepsilon\|_{L^\infty(0,\infty;H^{1,1}(\Omega))} + \|\tilde{\rho}^\varepsilon\|_{C^{1/13}([0,\infty);L^1(\Omega))} + \|\rho^\varepsilon\|_{C^{1/13}([0,\infty);L^2(\Omega))} \le C. \tag{3.17}$$

Proof. We take a smooth mollifier $\phi \in C^\infty(\mathbb{R}^d)$ such that $0 \le \phi \le 1, \int_{\mathbb{R}^d}\phi = 1, \operatorname{supp}(\phi) \subset B_1$ and define for $0 < \eta \le \eta_0$ for some $\eta_0 > 0$

$$\rho^\varepsilon_\eta(x,t) := \int_{B_1} \phi(y)\rho^\varepsilon(x-\eta y,t)dy = (-\eta)^{-d}\int_{\mathbb{R}^d}\phi(\tfrac{x-z}{\eta})\rho^\varepsilon(z,t)dz,$$

i.e. $\rho^\varepsilon_\eta = (-\eta)^{-d}(\phi \circ \frac{1}{\eta}) * \rho^\varepsilon$. The function ρ^ε is extended on $\mathbb{R}^d \setminus \Omega$ by zero (which is an arbitrary choice, just to have a well-defined ρ^ε). Note that the integration domain is still Ω and not some η-extension of Ω or even the whole $\mathbb{R}^d$. This means that the mass of mollified concentration function is partly smeared out of Ω and in general we don't have the equality $\int_\Omega \rho^\varepsilon = \int_\Omega \rho^\varepsilon_\eta$. Of course we do have the equality $\int_\Omega \rho^\varepsilon = \int_{\mathbb{R}^d}\rho^\varepsilon_\eta$.

(i) For the mollified concentration function ρ_η^ε we have the following estimates at all times t:

$$\|\nabla\rho_\eta^\varepsilon(.,t)\|_{L^2(\Omega)} \leq C\eta^{-1}\,\|\rho^\varepsilon(.,t)\|_{L^2(\Omega)} \leq C\eta^{-1},$$

since we have the a-priori estimate from Lemma 3.6 for the concentration function. The application of the chain rule on the mollified concentration function gives

$$\begin{aligned}\|\nabla\rho_\eta^\varepsilon(.,t)\|_{L^2(\Omega)} &= \eta^{-d}\int_\Omega |\nabla\big((\phi\circ\tfrac{1}{\eta})*\rho^\varepsilon\big)(x,t)|^2dx\\ &\leq \eta^{-d}\,\|\nabla(\phi\circ\tfrac{1}{\eta})\|_{L^1}\,\|\rho^\varepsilon(.,t)\|_{L^2}\\ &= \eta^{-d}\tfrac{1}{\eta}\eta^d\|\nabla\phi\|_{L^1}\|\rho^\varepsilon(.,t)\|_{L^2}\end{aligned}$$

by the estimates for mollified functions and the transformation rules for the gradient.

(ii) With the left side of (3.16) for the auxiliary function we get

$$\begin{aligned}\int_\Omega|\rho_\eta^\varepsilon-\rho^\varepsilon|^2 &\leq \int_\Omega\int_{B_1}\phi(y)|\rho^\varepsilon(x-\eta y,t)-\rho^\varepsilon(x,t)|^2dydx\\ &\leq \int_\Omega\int_{B_1}\phi(y)|\tilde\rho^\varepsilon(x-\eta y,t)-\tilde\rho^\varepsilon(x,t)|dydx\\ &= \int_\Omega\int_{B_1}\phi(y)\left|\int_0^1\nabla\tilde\rho^\varepsilon(x-\xi\eta y,t)\cdot\eta y\,d\xi\right|dydx\\ &\leq \eta\int_\Omega\int_{B_1}\int_0^1\phi(y)\,|\nabla\tilde\rho^\varepsilon(x-\xi\eta y,t)|\,d\xi dydx\\ &\leq \eta\int_{B_1}\int_0^1\phi(y)\int_\Omega|\nabla\tilde\rho^\varepsilon(x-\xi\eta y,t)|\,dxd\xi dy\\ &\overset{z=x-\xi\eta y}{\leq} C\eta\int_{B_1}\int_0^1\phi(y)\int_\Omega|\nabla\tilde\rho^\varepsilon(z,t)|\,dzd\xi dy\\ &= C\eta\int_\Omega|\nabla\tilde\rho^\varepsilon(z)|dz \leq C\eta\end{aligned}$$

for η small enough to make the translation of the integral $z = x - \xi\eta y$ valid. Here the function $\tilde\rho^\varepsilon$ is extended on $\mathbb{R}^d\setminus\Omega$ by zero as was ρ^ε.

(iii) Using the identity $\rho^\varepsilon(x,t)-\rho^\varepsilon(x,\tau) = \int_\tau^t\partial_t\rho^\varepsilon(x,s)ds$ in $H^{-1,2}(\Omega)$ (which follows for almost all $t,\tau > 0$ from the fundamental lemma of differential and integration calculus for Banach-space valued $H^{1,2}((0,T))$-functions), we can do the following calculations:

$$
\begin{aligned}
&\big\langle \rho^\varepsilon(t)-\rho^\varepsilon(\tau), \rho^\varepsilon_\eta(t)-\rho^\varepsilon_\eta(\tau)\big\rangle_{H^{1,2}(\Omega)}\\
&\qquad = \int_\tau^t \big\langle \partial_t\rho^\varepsilon(s), \rho^\varepsilon_\eta(t)-\rho^\varepsilon_\eta(\tau)\big\rangle_{H^{1,2}(\Omega)}\,ds\\
&\qquad \overset{(3.1)}{=} \int_\tau^t\int_\Omega \nabla w^\varepsilon(s,x)\cdot\nabla(\rho^\varepsilon_\eta(t,x)-\rho^\varepsilon_\eta(\tau,x))\,dx\,ds\\
&\qquad \overset{\text{Hölder-ineq.}}{\le} \|\nabla w^\varepsilon\|_{L^2(\Omega\times(t,\tau))}\|\nabla(\rho^\varepsilon_\eta(t,.)-\rho^\varepsilon_\eta(\tau,.))\|_{L^2(\Omega\times(t,\tau))}\\
&\qquad \overset{(1.63)}{\le} C\left(\int_\Omega |\nabla(\rho^\varepsilon_\eta(t,.)-\rho^\varepsilon_\eta(\tau,.))|^2\,dx\int_\tau^t 1\,ds\right)^{1/2}\\
&\qquad \overset{\text{cf.}(i)}{\le} C\,\eta^{-1}\,|t-\tau|^{1/2},
\end{aligned}
$$

since our test-function $\rho^\varepsilon_\eta(t)-\rho^\varepsilon_\eta(\tau)$ is fixed for the time integration variable, which is denoted here by s and has total mass zero.

(iv) Altogether we get

$$
\begin{aligned}
&\|\rho^\varepsilon(x,t)-\rho^\varepsilon(x,\tau)\|_{L^2(\Omega)}\\
&\quad = \big(\rho^\varepsilon(t)-\rho^\varepsilon(\tau), \rho^\varepsilon_\eta(t)-\rho^\varepsilon_\eta(\tau)\big)_{L^2(\Omega)}\\
&\qquad + \big(\rho^\varepsilon(t)-\rho^\varepsilon(\tau), \rho^\varepsilon(t)-\rho^\varepsilon_\eta(t)-(\rho^\varepsilon(\tau)-\rho^\varepsilon_\eta(\tau))\big)_{L^2(\Omega)}\\
&\quad \le \big(\rho^\varepsilon(t)-\rho^\varepsilon(\tau), \rho^\varepsilon_\eta(t)-\rho^\varepsilon_\eta(\tau)\big)_{L^2(\Omega)}\\
&\qquad + \|\rho^\varepsilon(t)-\rho^\varepsilon(\tau)\|^2_{L^2(\Omega)} + \tfrac{1}{2}\|\rho^\varepsilon(t)-\rho^\varepsilon_\eta(t)\|^2_{L^2(\Omega)} + \tfrac{1}{2}\|\rho^\varepsilon(\tau)-\rho^\varepsilon_\eta(\tau)|^2.
\end{aligned}
$$

With the result from point (ii) and point (iii) we can summarise

$$
\int_\Omega |\rho^\varepsilon(x,t)-\rho^\varepsilon(x,\tau)|^2dx \le C(\eta^{-1}|t-\tau|^{1/2}+\eta+\eta^{1/2}) \le C|t-\tau|^{1/6} \tag{3.18}
$$

for small $|t-\tau|$, if we choose $\eta = |t-\tau|^{1/3}$. This proves the third estimate of (3.17).

One remark on the change of scalar product of L^2 in point (iv) to the dual product of $H^{1,2}$ in point (iii) to get the estimate (3.18): The mapping $L^2 \to \mathbb{R}, \xi \mapsto (\rho^\varepsilon(t)-\rho^\varepsilon(\tau),\xi)_{L^2(\Omega)}$ can be read as an element of the dual space of $H^{1,2}(\Omega)$ (the well-posedness of this existence follows from the conservation of the total mass over time):

$$
\varrho \in H^{-1,2}(\Omega), \quad \varrho(\xi) := (\rho^\varepsilon(t)-\rho^\varepsilon(\tau),\xi)_{L^2(\Omega)}.
$$

This ϱ can be identified with $\int_\tau^t \partial_t\rho^\varepsilon ds$ as remarked above in point (iii).

The second estimate of (3.17) follows with the right side of (3.16)

$$\begin{aligned}\int_\Omega &|\tilde{\rho}^\varepsilon(x,t) - \tilde{\rho}^\varepsilon(x,\tau)|dx \\ &\leq C\|\rho^\varepsilon(.,t) - \rho^\varepsilon(.,\tau)\|_{L^2(\Omega)}\big(1 + \|\rho^\varepsilon(.,t)\|_{L^2(\Omega)} + \|\rho^\varepsilon(.,\tau)\|_{L^2(\Omega)}\big) \\ &\leq C(t-\tau)^{1/12},\end{aligned}$$

while the first estimate follows with (3.15). □

With these uniform bounds one can pass to the limit $\varepsilon \to 0$ along a sequence and together with Lemma 3.6 identify a set $M \subset \Omega \times [0,\infty)$ such that we have the following lemma:

Lemma 3.9. *For solutions of the Cahn-Larché system there exists a sequence $\varepsilon_j \to 0$ such that*

(i) $\tilde{\rho}^{\varepsilon_j}(x,t) \to 2\sigma\chi_M$ *in* $C^{1/13}([0,T];L^1(\Omega))$,

(ii) $\rho^{\varepsilon_j}(x,t) \to -1 + 2\chi_M$ *in* $C^{1/13}([0,T];L^2(\Omega))$ *and almost everywhere*

for all $T > 0$.

Proof. The estimate

$$\|\tilde{\rho}^\varepsilon\|_{L^\infty(0,\infty;H^{1,1}(\Omega))} < C < \infty$$

of Lemma 3.8 shows by compactness of $BV(\Omega)$ that for almost all times $t > 0$ we have a limit $\tilde{\rho}^\varepsilon_t \in BV(\Omega)$ along a sequence $\varepsilon_j \to 0$. If we look at the respective ρ_t according to (3.14), we know with the third estimate from Lemma 3.6 that ρ_t has values only in $\{\pm 1\}$. Reconsidering that $\tilde{\rho}^\varepsilon_t \in BV(\Omega)$ there has to be a set M_t of bounded perimeter such that

$$\tilde{\rho}^{\varepsilon_j}(t,.) \to 2\sigma\chi_{M_t} \quad \text{and} \quad \rho^{\varepsilon_j}(t,.) \to -1 + 2\chi_{M_t} \tag{3.19}$$

for almost every $t > 0$. Using the 2nd and 3rd estimate of Lemma 3.8 and Theorem A.2 we obtain the continuity in time. □

The set M defines $\Omega_+(t)$ for all $t > 0$.

This proves the first convergence statement of the Proposition 3.2.

3.2.4 Convergence of deformation

Set $\Omega_T := (0,T) \times \Omega$.

Lemma 3.10. *The strain tensor is uniformly bounded in $\varepsilon > 0$:*

$$\|\mathcal{E}(\mathbf{u}^\varepsilon)\|_{L^2(\Omega_T)} \leq C \tag{3.20}$$

Proof. Using the monotonicity of $W_{,\mathcal{E}}$, see (1.5), we obtain that the elastic energy density fulfils

$$W(\rho, \mathcal{E}) \geq C_0|\mathcal{E}|^2 - C_1(|\rho|^2 + 1)$$

for some constants $C_0, C_1 > 0$. Therefore we have for solutions $(\rho^\varepsilon, \mathbf{u}^\varepsilon)$

$$\int_{\Omega_T} |\mathcal{E}(\mathbf{u}^\varepsilon)|^2 \, dx \, dt \leq C \left(1 + \int_{\Omega_T} W(\rho^\varepsilon, \mathcal{E}(\mathbf{u}^\varepsilon)) \, dx \, dt + \int_{\Omega_T} |\rho^\varepsilon|^2 \, dx \, dt \right) \leq C(1 + \mathbf{E}_0).$$

Since the W-term is bounded by the total energy $\mathbf{E}^\varepsilon_{\mathbf{pf}}$ and the ρ^ε-term by the a priori estimate in Lemma 3.6, we have that $\|\mathcal{E}(\mathbf{u}^\varepsilon)\|_{H^{1,2}(\Omega_T)}$ is bounded uniformly in t and ε. □

By Korn's inequality, see appendix A.3, we can thereby control the deformation vector $\mathbf{u}^\varepsilon$ in $L^2(0, T; \mathrm{X}_{\mathrm{ird}})$:

Lemma 3.11.

$$\int_0^T \|\mathbf{u}^\varepsilon\|^2_{H^{1,2}(\Omega)} \leq C \int_{\Omega_T} |\mathcal{E}(\mathbf{u}^\varepsilon)|^2 \, dx \, dt \leq C. \tag{3.21}$$

Lemma 3.12. *The sequence $\mathbf{u}^\varepsilon$ converges strongly in $L^2(0, T; H^{1,2}(\Omega, \mathbb{R}^d))$.*

Proof. Since $L^2(0, T; H^{1,2}(\Omega, \mathbb{R}^d))$ is a Hilbert-space, thus a reflexive space, we conclude the weak compactness of the deformation vector functions, i.e. there exists a $\mathbf{u} \in L^2(0, T; H^{1,2}(\Omega, \mathbb{R}^d))$ such that for all sequences $(\varepsilon_j)_{j\in\mathbb{N}}$ there exists a subsequence $(\varepsilon_{j_k})_{k\in\mathbb{N}}$ such that

$$\mathbf{u}^{\varepsilon_{j_k}} \to \mathbf{u} \quad \text{weakly in } L^2(0, T; H^{1,2}(\Omega, \mathbb{R}^d))$$

Once more, we use the monotonicity of $W_{,\mathcal{E}}$ to get

$$\begin{aligned} c_1\|\mathcal{E}(\mathbf{u}^\varepsilon - \mathbf{u})\|^2_{L^2(\Omega_T)} &\leq \int_{\Omega_T} \big(W_{,\mathcal{E}}(\rho^\varepsilon, \mathcal{E}(\mathbf{u}^\varepsilon)) - W_{,\mathcal{E}}(\rho^\varepsilon, \mathcal{E}(\mathbf{u}))\big) : \mathcal{E}(\mathbf{u}^\varepsilon - \mathbf{u}) \\ &= -\int_{\Omega_T} W_{,\mathcal{E}}(\rho^\varepsilon, \mathcal{E}(\mathbf{u})) : \mathcal{E}(\mathbf{u}^\varepsilon - \mathbf{u}). \end{aligned} \tag{3.22}$$

The last equality is due to the divergence free stress tensor, cf. equation (1.62). One should notice that only $W_{,\mathcal{E}}(\rho^\varepsilon, \mathcal{E}(\mathbf{u}^\varepsilon))$, but not $W_{,\mathcal{E}}(\rho^\varepsilon, \mathcal{E}(\mathbf{u}))$ is divergence free, since only in the first term the respective deformation field $\mathbf{u}^\varepsilon$ meets the condition (1.62). Note also that from the same equation we also have

$$\begin{aligned} 0 &= \int W_{,\mathcal{E}}(\rho^\varepsilon, \mathcal{E}(\mathbf{u}^\varepsilon)) : \nabla\eta = \int \sum_{ij} W_{,\mathcal{E}_{ij}}(\rho^\varepsilon, \mathcal{E}(\mathbf{u}^\varepsilon))\partial_i\eta_j \\ &= \int \sum_{ij} W_{,\mathcal{E}_{ji}}(\rho^\varepsilon, \mathcal{E}(\mathbf{u}^\varepsilon))\partial_i\eta_j = \int W_{,\mathcal{E}}(\rho^\varepsilon, \mathcal{E}(\mathbf{u}^\varepsilon)) : (\nabla\eta)^T. \end{aligned}$$

By the strong convergence of the concentration function and the weak convergence of the deformation field, the right hand side of equation (3.22) goes to zero, i.e. we obtain strong convergence of the strain tensor for the sequence $(\varepsilon_{j_k})_{k\in\mathbb{N}}$. By Korn's inequality the deformation vector converges strongly in $L^2(0,T;H^{1,2}(\Omega,\mathbb{R}^d))$. In particular we have that $\nabla\mathbf{u}^{\varepsilon_{j_k}}(t)$ converges strongly to $\nabla\mathbf{u}(t)$ in $L^2(\Omega)$ for almost all t. □

This verifies the third convergence statement of the Proposition 3.2.

3.2.5 Convergence of chemical potential

First, we derive an $H^{1,2}(\Omega)$ estimate for the chemical potential w^ε for almost every time t. We will then see that this carries further to a time-space estimate of $L^2(0,T;H^{1,2}(\Omega))$-type, so that compactness of w^ε is obtained.

We begin with the following Poincaré type inequality:

Lemma 3.13. *For the solutions of the Cahn-Larché system we obtain*

$$\|w^\varepsilon(.,t)\|_{H^{1,2}(\Omega)} \le C(\mathbf{E}^\varepsilon_{\mathbf{pf}}(t) + \|\nabla w^\varepsilon(.,t)\|_{L^2(\Omega)}) \tag{3.23}$$

for almost every time $t>0$.

Proof. We first localise equation (3.2) in time as we did in Subsection 1.4.1. So we can use equation (1.74) instead of (3.2) and get with test-function $\vec{X}\cdot\nabla\rho^\varepsilon$ for $\vec{X}\in C^1(\Omega,\mathbb{R}^d)$ with boundary values $\vec{X}\cdot\nu_\Omega = 0$:

$$\begin{aligned}\int w^\varepsilon\vec{X}\cdot\nabla\rho^\varepsilon &= \int \varepsilon\nabla\rho^\varepsilon\cdot\nabla(\vec{X}\cdot\nabla\rho^\varepsilon) + \tfrac{1}{\varepsilon}\Psi'(\rho^\varepsilon)\vec{X}\cdot\nabla\rho^\varepsilon + W_{,\rho}(\rho^\varepsilon,\mathcal{E}(\mathbf{u}^\varepsilon))\vec{X}\cdot\nabla\rho^\varepsilon\\ &= \int \varepsilon\left(\nabla\rho^\varepsilon\cdot D\vec{X}\nabla\rho^\varepsilon - \tfrac{1}{2}\operatorname{div}\vec{X}\,|\nabla\rho^\varepsilon|^2\right) + (\tfrac{1}{\varepsilon}\Psi' + W_{,\rho})\vec{X}\cdot\nabla\rho^\varepsilon.\end{aligned}$$

Now we see that via partial integration – the boundary integrals vanish by the choice of test functions

$$\int D\vec{X} : (\Psi\,\mathbf{id}) = \int \operatorname{div}\vec{X}\,\Psi = -\int \vec{X}\cdot\nabla\rho^\varepsilon\,\Psi' \tag{3.24}$$

and

$$\int D\vec{X} : (W\,\mathbf{id}) = \int \operatorname{div}\vec{X}\,W = -\int \vec{X}\cdot\nabla\rho^\varepsilon\,W_{,\rho} + \vec{X}_i W_{,\mathcal{E}_{kl}}\partial_i\partial_k\mathbf{u}^\varepsilon_l \tag{3.25}$$

$$= -\int \vec{X}\cdot\nabla\rho^\varepsilon W_{,\rho} - (\partial_k\vec{X}_i)W_{,\mathcal{E}_{kl}}\partial_i\mathbf{u}^\varepsilon_l, \tag{3.26}$$

where we used equation (3.3). With $W_{,\mathcal{E}_{kl}} = S_{kl}$ we obtain

$$\int \operatorname{div}(w^\varepsilon\vec{X})\rho^\varepsilon = \int D\vec{X} : \left[e^\varepsilon(\rho^\varepsilon)\,\mathbf{id} - \varepsilon\nabla\rho^\varepsilon\otimes\nabla\rho^\varepsilon + W\,\mathbf{id} - (\nabla\mathbf{u}^\varepsilon)^T S\right]. \tag{3.27}$$

We now introduce the mean value of w^ε as $\bar{w}^\varepsilon$ and use integration by parts to obtain

$$\int_\Omega w^\varepsilon\vec{X}\cdot\nabla\rho^\varepsilon = -\int_\Omega \nabla w^\varepsilon\cdot\vec{X}\rho^\varepsilon - \int_\Omega (w^\varepsilon - \bar{w}^\varepsilon)\rho^\varepsilon\operatorname{div}\vec{X} - \bar{w}^\varepsilon\int_\Omega \rho^\varepsilon\operatorname{div}\vec{X}. \tag{3.28}$$

Combining equation (3.27) and (3.28), one arrives at

$$\bar{w}^\varepsilon = \frac{1}{\int_\Omega \rho^\varepsilon \operatorname{div} \vec{X}} \int_\Omega D\vec{X} : \left[(e^\varepsilon(\rho^\varepsilon) + W(\rho^\varepsilon, \mathcal{E}(\mathbf{u}^\varepsilon)))\, \mathbf{id} - \varepsilon \nabla\rho^\varepsilon \otimes \nabla\rho^\varepsilon - (\nabla \mathbf{u}^\varepsilon)^T S \right]$$

$$- \nabla w^\varepsilon \cdot \vec{X}\rho^\varepsilon - (w^\varepsilon - \bar{w}^\varepsilon)\rho^\varepsilon \operatorname{div} \vec{X}\, dx. \tag{3.29}$$

Now, we choose a more specific test function: $\vec{X} = \nabla Y$ shall be such that Y is the solution of

$$-\Delta Y = \rho_\eta^\varepsilon - \left(\int_\Omega \rho_\eta^\varepsilon \right) \qquad \text{in } \Omega, \tag{3.30}$$

$$\nabla Y \cdot \nu_\Omega = 0 \qquad \text{on } \partial\Omega \tag{3.31}$$

$$\text{and } \int_\Omega Y = 0. \tag{3.32}$$

Here ρ_η^ε is the mollified concentration function for $\eta > 0$ as in the proof of Lemma 3.8. The integral on the right side is subtracted to guarantee the well-posedness of the problem.

By the definition of ρ_η^ε in Lemma 3.8 we can make the following estimates

$$\begin{aligned}
\|\rho_\eta^\varepsilon\|_{L^\infty(\Omega)} &= \sup_{x\in\Omega} \left| (-\eta)^{-d} \int_{\mathbb{R}^d} \phi(\tfrac{x-y}{\eta}) \rho^\varepsilon(y) dy \right| \\
&\le 1 + \eta^{-d} \sup_{x\in\Omega} \int_{\mathbb{R}^d} \phi(\tfrac{x-y}{\eta}) \big| |\rho^\varepsilon(y)| - 1 \big| dy \\
&\le 1 + \eta^{-d} \| |\rho^\varepsilon(y)| - 1 \|_{L^2(\Omega)} \sup_{x\in\Omega} \left(\int_{\mathbb{R}^d} \phi^2(\tfrac{x-y}{\eta}) dy \right)^{1/2} \\
&\le 1 + \eta^{-d} C\sqrt{\varepsilon}\, C\, \eta^{d/2} = 1 + C\, \eta^{-d/2}\sqrt{\varepsilon}
\end{aligned}$$

and since $\partial_i(\phi * \rho^\varepsilon) = (\partial_i\phi) * \rho^\varepsilon$ we get similarly

$$\begin{aligned}
\|\rho_\eta^\varepsilon\|_{C^1(\Omega)} &= \sup_{x\in\Omega, i\in\{1,\ldots,n\}} \left| (-\eta)^{-d} \int_{\mathbb{R}^d} \partial_{x_i}\phi(\tfrac{x-y}{\eta}) \rho^\varepsilon(y) dy \right| \\
&= \sup_{x\in\Omega, i\in\{1,\ldots,n\}} \left| (-\eta)^{-d} \int_{\mathbb{R}^d} \partial_{x_i}\phi(\tfrac{x-y}{\eta}) \left(\rho^\varepsilon(y) - 1\right) dy \right| \\
&\le \eta^{-d} \| |\rho^\varepsilon(y)| - 1 \|_{L^2(\Omega)} \sup_{x\in\Omega} \left(\int_{\mathbb{R}^d} (\partial_{x_i}\phi)^2(\tfrac{x-y}{\eta}) dy \right)^{1/2} \\
&\le C\eta^{-d}\sqrt{\varepsilon}\, \eta^{(d-2)/2} \le C\eta^{-d/2-1}\sqrt{\varepsilon}.
\end{aligned}$$

Using the elliptic estimate (see for instance Chapter 4 in [DauLio90], where the C^2-regularity results from [GilTru98] are adapted to the Neumann boundary case) we get with

$$\|Y\|_{C^2(\Omega)} \le C \left(\|\rho_\eta^\varepsilon\|_{C^0(\Omega)} + \|\rho_\eta^\varepsilon\|_{C^1(\Omega)} \right) \le C(1 + \eta^{-d/2-1}\sqrt{\varepsilon})$$

an upper bound for the numerator of (3.29):

$$\begin{aligned}\int_\Omega \Big(D\vec{X} : \big[(e^\varepsilon(\rho^\varepsilon) + W(\rho^\varepsilon, \mathbf{u}^\varepsilon))\,\mathbf{id} - \varepsilon\nabla\rho^\varepsilon \otimes \nabla\rho^\varepsilon - (\nabla\mathbf{u}^\varepsilon)^T S\big] \\ - \nabla w^\varepsilon \cdot \vec{X}\rho^\varepsilon - (w^\varepsilon - \bar{w}^\varepsilon)\rho^\varepsilon \operatorname{div}\vec{X}\Big)\,dx \\ \le C\|Y\|_{C^2(\Omega)}\big(\mathbf{E}^\varepsilon_{\mathbf{pf}}(t) + \|(\nabla\mathbf{u}^\varepsilon)^T S\|_{L^1(\Omega)} + \|\rho^\varepsilon\|_{L^2(\Omega)}\|\nabla w^\varepsilon\|_{L^2(\Omega)} \\ + \|\rho^\varepsilon\|_{L^2(\Omega)}\|w^\varepsilon - \bar{w}^\varepsilon\|_{L^2(\Omega)}\big)\end{aligned}$$

Here, we need

$$\begin{aligned}\int_\Omega \big|(\nabla\mathbf{u}^\varepsilon)^T S\big| &\le \|\nabla\mathbf{u}^\varepsilon\|_{L^2(\Omega)}\left(\int_\Omega |S|^2\right)^{1/2} \\ &\le C\|\mathbf{u}^\varepsilon\|_{H^{1,2}(\Omega)}\left(\int_\Omega (|\mathcal{E}(\mathbf{u}^\varepsilon)| + |\rho^\varepsilon| + 1)^2\right)^{1/2} \\ &\le C\|\mathbf{u}^\varepsilon\|_{H^{1,2}(\Omega)}(\|\mathbf{u}^\varepsilon\|_{H^{1,2}(\Omega)} + \|\rho^\varepsilon\|_{L^2(\Omega)} + 1).\end{aligned}$$

Now, for the denominator $\int \rho^\varepsilon \operatorname{div}\vec{X}$ we insert some Null-terms to come out with

$$\begin{aligned}\int \rho^\varepsilon \operatorname{div}\vec{X} &= \int \left(\rho^\varepsilon_\eta - \bar{\rho}^\varepsilon_\eta\right)\rho^\varepsilon \\ &= \int \left[\left(\rho^\varepsilon_\eta - \rho^\varepsilon\right)\rho^\varepsilon + (\rho^\varepsilon)^2 - 1\right] + |\Omega|(1 - \bar{\rho}^{\varepsilon 2}) + |\Omega|\bar{\rho}^\varepsilon(\bar{\rho}^\varepsilon - \bar{\rho}^\varepsilon_\eta).\end{aligned}$$

Then we can use the estimates from the proof of Lemma 3.8:

$$\left|\bar{\rho}^\varepsilon - \bar{\rho}^\varepsilon_\eta\right| = \frac{1}{|\Omega|}\left|\int_\Omega \rho^\varepsilon - \rho^\varepsilon_\eta\right| \le C\|\rho^\varepsilon - \rho^\varepsilon_\eta\|_{L^2(\Omega)} \le C\sqrt{\eta}$$

and

$$\int \left(\rho^\varepsilon_\eta - \rho^\varepsilon\right)\rho^\varepsilon \le \|\rho^\varepsilon_\eta - \rho^\varepsilon\|_{L^2(\Omega)}\|\rho^\varepsilon\|_{L^2(\Omega)} \le C\sqrt{\eta}\,C.$$

Since $\bar{\rho}^\varepsilon = \frac{m_0}{|\Omega|}$ and by estimate 3 of Lemma 3.6, we get altogether

$$\int \rho^\varepsilon \operatorname{div}\vec{X} \ge |\Omega|(1 - m_0^2) - C(\sqrt{\varepsilon} + \sqrt{\eta}). \tag{3.33}$$

The mean concentration m_0 is between -1 and 1, so if we choose a small $\eta > 0$ and restrict $\varepsilon > 0$ to a sufficiently small range, the denominator stays uniformly positive and we have an estimate for the mean value of the potential function:

$$|\bar{w}^\varepsilon| \le C(1 + \eta^{-d/2-1}\sqrt{\varepsilon})\left(\mathbf{E}^\varepsilon_{\mathbf{pf}}(t) + C + \|\nabla w^\varepsilon\|_{L^2(\Omega)}\right) \tag{3.34}$$

by the estimates of the previous subsections.

Using the generalised Poincaré-inequality, this yields a uniform estimate for the chemical potential $\|w^\varepsilon\|_{H^{1,2}(\Omega)}$ which concludes the proof. □

With this bound we also have a $L^2(0,T;H^{1,2}(\Omega))$ bound, since the right hand side of (3.23) is $L^2(0,T)$-integrable. So we can conclude the weak convergence of the chemical potential.

Corollary 3.14. *There exist constants $C, \varepsilon_0 > 0$ such that for all $\varepsilon \in (0, \varepsilon_0]$ and all $T > 0$ it holds*

$$\int_0^T \|w^\varepsilon(.,t)\|^2_{H^{1,2}(\Omega)} \leq C. \tag{3.35}$$

Therefore, for a sequence $\varepsilon_j \to 0$ there exists a function $w \in L^2(0,T;H^{1,2}(\Omega))$ such that

$$w^{\varepsilon_j} \to w \qquad \text{weakly in } L^2(0,T;H^{1,2}(\Omega)).$$

Proof. This is an immediate consequence of Lemma 1.4, as the right side of (3.23) is $L^2(0,T)$-integrable. We remark that $L^2(0,T;H^{1,2}(\Omega))$ is a reflexive Banach space. □

3.2.6 Radon measures as limit interfaces

The Gibbs-Thomson law is expressed using ideas of geometric measure theory. It turns out that the notion of varifolds is appropriate to describe the curvature term in a sufficiently general way and incorporates a very useful compactness property, see Theorem 2.9. Generally the idea would be to apply the compactness property of varifolds 2.9 for the phase-field solutions considered as varifolds and observe the limit $\varepsilon \to 0$. Here we directly calculate V and represent them via the Radon measures μ, μ_{ij}. The subsequent Subsection 3.2.7 verifies that these Radon measures do give rise to a varifold.

The energy density $e^\varepsilon(\rho^\varepsilon) := \frac{\varepsilon}{2}|\nabla\rho^\varepsilon|^2 + \frac{1}{\varepsilon}\Psi(\rho^\varepsilon)$ and $\varepsilon\nabla\rho^\varepsilon \otimes \nabla\rho^\varepsilon$ are bounded by the initial energy:

$$\int_0^T \int_\Omega e^\varepsilon(\rho^\varepsilon)\,dx\,dt \leq \int_0^T \mathbf{E}^\varepsilon_{\mathbf{pf}}(t)\,dt \leq T\mathbf{E}_0$$

$$\int_0^T \int_\Omega \varepsilon \left|\partial_{x_i}\rho^\varepsilon\,\partial_{x_j}\rho^\varepsilon\right|\,dx\,dt \leq 2\int_0^T \int_\Omega e^\varepsilon(\rho^\varepsilon)\,dx\,dt \leq 2T\mathbf{E}_0.$$

We can take these integral expressions as Radon measures: $\mu^\varepsilon(A) := \int_A e^\varepsilon(\rho^\varepsilon)\,dxdt$ and $\mu^\varepsilon_{ij}(A) := \int_A \varepsilon(\partial_{x_i}\rho^\varepsilon)\,(\partial_{x_j}\rho^\varepsilon)\,dxdt$ for Borel sets $A \subset \Omega \times [0,T]$. Here μ^ε_{ij} is a signed measure, but due their representation via L^1-functions, they are Borel regular, i.e. Radon measures.

By compactness of Radon measures there exist Radon measures μ and μ_{ij} according to (3.7) and (3.8). Furthermore we can split them into a spatial and time part.

Proposition 3.15. *The Radon measures $d\mu(x,t)$ and $d\mu_{ij}(x,t)$ from above have representation by a spatial and time component:*

$$d\mu(x,t) = d\mu^t(x)\,dt, \qquad d\mu_{ij}(x,t) = d\mu^t_{ij}(x)\,dt \tag{3.36}$$

such that μ^t, μ^t_{ij} for $i,j \in \mathbb{N}$ are Radon measures on Ω.

Proof. This follows from the disintegration theorem A.6. We can rescale the measures so that they are probability measures and choose the projection $\pi\colon [0,T]\times\bar{\Omega}\to[0,T]$. The application of the disintegration theorem results in the existence of probability measures $\pi_\sharp\mu(t)$ and $\mu^t(x)$ which in our case are Radon measures, see Proposition A.7. Since our time interval $[0,T]$ is armed with the usual 1-dimensional Lebesgue measure and since the push-forward $\pi_\sharp\mu$ is Borel regular, it is a Radon measure and we have the decomposition with respect to dt:

$$d(\pi_\sharp\mu)(t) = \pi_\sharp\mu_{\mathsf{ac}}(t)\,dt + d(\pi_\sharp\mu_{\mathsf{sing}})(t) \tag{3.37}$$

where the $\pi_\sharp\mu_{\mathsf{ac}}\in L^1(dt)$ is the Radon-Nikodym derivative of $\pi_\sharp\mu$ with respect to time and $\pi_\sharp\mu_{\mathsf{sing}}$ the singular part. We now claim that $\pi_\sharp\mu_{\mathsf{sing}}$ is in fact zero. We show that μ is absolutely continuous in time:

$$\mu(O\times E)\to 0 \text{ whenever } |E|\to 0 \text{ with measurable } E\subset[0,T] \tag{3.38}$$

for all measurable $O\subset\Omega$. This follows by the respective continuity of the phase-field energy:

$$\begin{aligned}
\mu(O\times E) &= \lim_{\varepsilon\to 0}\int_E\int_O e^\varepsilon(\rho^\varepsilon)(t,x)\,dx\,dt\\
&\le \lim_{\varepsilon\to 0}\int_E\int_\Omega e^\varepsilon(\rho^\varepsilon)(t,x)\,dx\,dt\\
&\le \lim_{\varepsilon\to 0}\int_E \mathbf{E}^0\,dt\\
&= \mathbf{E}^0\,|E|.
\end{aligned}$$

So $\pi_\sharp\mu$ is in fact absolutely continuous with respect to dt and therefore the singular part $\pi_\sharp\mu_{\mathsf{sing}}$ must vanish and we have the identity

$$d\mu(x,t) = \tilde{\mu}^t(x)\,\pi_\sharp\mu_{\mathsf{ac}}\,dt$$

where $\tilde{\mu}^t$ is the time dependent Radon measure on Ω which corresponds to μ_y in the notation of the disintegration theorem A.6. After rescaling $\tilde{\mu}^t$ by l_μ we can get our splitting (3.36) for μ. For the signed measures μ_{ij} we repeat the same procedure for both positive and negative part respectively

$$\mu_{ij} = \mu_{ij}^+ - \mu_{ij}^-.$$

□

The energy estimates in Lemma 1.4 show that the energies of the phase-field solutions are non-increasing. For the limit sharp-interface model we can identify an energy function with a similar dissipation inequality.

Lemma 3.16. *For a sequence $\varepsilon_k \to 0$ there exists a non-negative, non-increasing function $\mathbf{E_{si}}\colon [0,\infty) \to [0,\infty)$ such that for almost all $t > 0$*

$$\mathbf{E}_{\mathbf{pf}}^{\varepsilon_k}(t) \to \mathbf{E_{si}}(t).$$

Moreover this function can be identified with

$$\mathbf{E_{si}}(t) = \mu^t(\Omega) + \int_\Omega \sum_{k=\pm 1} W(k, \mathcal{E}(\mathbf{u}(t,.))) \tag{3.39}$$

and the dissipation estimate

$$\mathbf{E_{si}}(t) + \int_0^t \int_\Omega |\nabla w|^2 \leq \mathbf{E_{si}}(0) \leq \mathbf{E}_0 \tag{3.40}$$

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

Remark. This shows that property (iv) of definition of a generalised solution 3.1 is fulfilled in the limit $\varepsilon \to 0$.

Proof. The functions $\mathbf{E}_{\mathbf{pf}}^{\varepsilon}$ are bounded uniformly in $\varepsilon > 0$ and $t > 0$. Therefore along a sequence $\varepsilon_k \to 0$ for almost every $t \in [0,T]$ there exists the pointwise limit

$$\lim_{\varepsilon_k \to 0} \mathbf{E}_{\mathbf{pf}}^{\varepsilon_k}(t) =: \mathbf{E_{si}}(t). \tag{3.41}$$

The monotonicity of $\mathbf{E}_{\mathbf{pf}}^{\varepsilon}$ carries through the limit, so that $\mathbf{E_{si}}$ is a monotone function with the same bounds:

$$0 \leq \mathbf{E_{si}}(t) \leq \mathbf{E}_0 \qquad \forall\, t \in [0,T].$$

As a monotone, bounded function it can have at most countable many jumps and is continuous everywhere else. Recall the energy of the phase-field model:

$$\begin{aligned}\mathbf{E}_{\mathbf{pf}}^{\varepsilon}(\rho^\varepsilon, \mathbf{u}^\varepsilon) &= \int_\Omega \frac{\varepsilon}{2}|\nabla \rho^\varepsilon|^2 + \frac{1}{\varepsilon}\Psi(\rho^\varepsilon) + W(\rho^\varepsilon, \mathcal{E}(\mathbf{u}^\varepsilon)) \\ &= \int_\Omega e^\varepsilon(\rho^\varepsilon) + W(\rho^\varepsilon, \mathcal{E}(\mathbf{u}^\varepsilon))\end{aligned}$$

Now, we take a dense, countable subset $\mathcal{T} = \{t_k \mid k \in \mathbb{N}\}$ of the time interval $[0,T]$. Since the energy is uniformly bounded by $\mathbf{E}_0$ for $\varepsilon > 0$ and $t \in [0,T]$, we can find through a diagonal argument a subsequence $\varepsilon_l \to 0$ of $(\varepsilon_k)_k$ such that

$$\int_\Omega e^{\varepsilon_l}(\rho^{\varepsilon_l}(t_k,.)) \to \mathfrak{m}(t_k) \tag{3.42}$$

for all $t_k \in \mathcal{T}$ as $\varepsilon_l \to 0$ for some non-negative function $t \mapsto \mathfrak{m}(t)$ which we expect to be $\mu^t(\Omega)$. For the remaining part we just use the last sequence $(\varepsilon_l)_{l\in\mathbb{N}}$.

For $t \in [0,T] \setminus \mathcal{T}$ such that (3.41) holds and $\mathbf{E_{si}}$ is continuous in t we claim that we have a limit function $\lim_{t_k \to t} \mathfrak{m}(t_k)$:

$$\lim_{\varepsilon_l \to 0} \int_\Omega e^{\varepsilon_l}(\rho^{\varepsilon_l}(t)) = \lim_{t_k \to t} \mathfrak{m}(t_k) =: \mathfrak{m}(t). \tag{3.43}$$

- For any $t_k \in \mathcal{T}, t_k > t$ the following holds

$$\begin{aligned}
&\liminf_{\varepsilon_l \to 0} \int_\Omega e^{\varepsilon_l}(\rho^{\varepsilon_l}(t)) \\
&\qquad = \liminf_{\varepsilon_l \to 0} \int_\Omega e^{\varepsilon_l}(\rho^{\varepsilon_l}(t)) + \int_\Omega W(\rho^{\varepsilon_l}(t), \mathcal{E}(\mathbf{u}^{\varepsilon_l}(t))) - \int_\Omega W(\rho^{\varepsilon_l}(t), \mathcal{E}(\mathbf{u}^{\varepsilon_l}(t))) \\
&\qquad = \liminf_{\varepsilon_l \to 0} \mathbf{E}^{\varepsilon_l}_{\mathbf{pf}}(t) - \int_\Omega W(\rho^{\varepsilon_l}(t), \mathcal{E}(\mathbf{u}^{\varepsilon_l}(t))) \\
&\qquad \geq \liminf_{\varepsilon_l \to 0} \mathbf{E}^{\varepsilon_l}_{\mathbf{pf}}(t_k) - \int_\Omega W(\rho^{\varepsilon_l}(t), \mathcal{E}(\mathbf{u}^{\varepsilon_l}(t))) \\
&\qquad = \mathbf{E_{si}}(t_k) - \int_\Omega W(-1 + 2\chi_{M^t}, \mathcal{E}(\mathbf{u}(t))).
\end{aligned}$$

By the choice of t the energy $\mathbf{E_{si}}$ is continuous in t and we have therefore by letting $t_k \searrow t$

$$\liminf_{\varepsilon_l \to 0} \int_\Omega e^{\varepsilon_l}(\rho^{\varepsilon_l}(t)) \geq \mathbf{E_{si}}(t) - \int_\Omega W(-1 + 2\chi_{M^t}, \mathcal{E}(\mathbf{u}(t))). \tag{3.44}$$

- If we now use the analogue argument as above with $t_k \in \mathcal{T}, t_k < t$, we get

$$\limsup_{\varepsilon_l \to 0} \int_\Omega e^{\varepsilon_l}(\rho^{\varepsilon_l}(t)) \leq \mathbf{E_{si}}(t_k) - \int_\Omega W(-1 + 2\chi_{M^t}, \mathcal{E}(\mathbf{u}(t)))$$

and therefore by letting $t_k \nearrow t$

$$\limsup_{\varepsilon_l \to 0} \int_\Omega e^{\varepsilon_l}(\rho^{\varepsilon_l}(t)) \leq \mathbf{E_{si}}(t) - \int_\Omega W(-1 + 2\chi_{M^t}, \mathcal{E}(\mathbf{u}(t))). \tag{3.45}$$

The limits (3.44) and (3.45) yield

$$\lim_{\varepsilon_l \to 0} \int_\Omega e^{\varepsilon_l}(\rho^{\varepsilon_l}(t)) = \mathbf{E_{si}}(t) - \int_\Omega W(-1 + 2\chi_{M^t}, \mathcal{E}(\mathbf{u}(t))). \tag{3.46}$$

Since the term $\int_\Omega W(\rho^{\varepsilon_l}(t), \mathcal{E}(\mathbf{u}^{\varepsilon_l}(t)))$ converges for almost every $t \in [0,T]$ by the strong convergences of the concentration function in $L^2(\Omega)$ and of the deformation vector in $H^{1,2}(\Omega)$, we arrive at

$$\lim_{\varepsilon_l \to 0} \int_\Omega e^{\varepsilon_l}(\rho^{\varepsilon_l}(t)) \to \mathfrak{m}(t) = \mu^t(\Omega). \tag{3.47}$$

Note that for almost all $t \in [0,T]$ the restrictions in the claim of (3.43) are fulfilled. Therefore (3.47) holds for almost every $t \in [0,T]$. □

Remark. Note that the function $\mathbf{E_{si}}$ can have (countably many) discontinuities. This reflects the change of the number of particles, i.e. the change of topology. The reason is that within a time period of stable topology the energy changes only smoothly, cf. [LuStu95] for such type of evolutions, see also remarks in Subsection 3.3.

3.2.7 Identifying the varifold

So far, we have shown the convergences as stated in the theorem, but we still have to verify, if the limit functions do represent a generalised solution according to Definition 3.1. Indeed the first diffusion equation immediately follows from equation (3.1) and the convergences of the concentration function and potential. The identity (v) in Definition 3.1 follows from (3.3) in the limit $\varepsilon \to 0$, as $\nabla \mathbf{u}^\varepsilon$ and ρ^ε converge strongly. The other conditions require the specification of the varifold. With the above-mentioned convergences we want to know what kind of equations for the limit functions hold.

The latter part deals with the limit varifold V. It is mainly derived from the convergence mentioned in the second part of the Proposition 3.2 and we show the remaining conditions of Definition 3.1 assuming that Theorem 3.4 holds. Equation (3.27) gives in the limit $\varepsilon \to 0$

$$\int_\tau^t \int_\Omega 2\chi_{\Omega_-} \operatorname{div}(w\vec{X}) = \int_\tau^t \int_\Omega D\vec{X} : [d\mu \, \mathbf{id} - (d\mu_{ij})_{ij}] + \int_\tau^t \int_\Omega D\vec{X} : (W \, \mathbf{id} - (\nabla \mathbf{u})^T S). \tag{3.48}$$

We claim now that $\int D\vec{X} : [d\mu \, \mathbf{id} - (d\mu_{ij})_{ij}]$ can be seen as the first variation of a varifold. This will prove Proposition 3.3. Furthermore, property (ii) of the definition of a generalised solution 3.1 will be verified. Before proving Proposition 3.3 we need the following estimate:

Lemma 3.17. *For $\vec{Y}, \vec{Z} \in C^0(\bar{\Omega} \times [0,T], \mathbb{R}^d)$ one has*

$$\int_0^T \int_\Omega \vec{Y}^T (\varepsilon \nabla \rho^\varepsilon \otimes \nabla \rho^\varepsilon) \vec{Z} \le \int_0^T \int_\Omega |\vec{Y}||\vec{Z}| e^\varepsilon(\rho^\varepsilon) + \int_0^T \int_\Omega |\vec{Y}||\vec{Z}| \xi^\varepsilon(\rho^\varepsilon). \tag{3.49}$$

Proof. This follows simply by

$$\begin{aligned} \vec{Y}^T (\varepsilon \nabla \rho^\varepsilon \otimes \nabla \rho^\varepsilon) \vec{Z} &\le \left| \vec{Y}^T (\varepsilon \nabla \rho^\varepsilon \otimes \nabla \rho^\varepsilon) \vec{Z} \right| \\ &\le |\vec{Y}| \, |\vec{Z}| \, \|\varepsilon \nabla \rho^\varepsilon \otimes \nabla \rho^\varepsilon\| \le |\vec{Y}| \, |\vec{Z}| \, \varepsilon \|\nabla \rho^\varepsilon\|^2 \\ &= |\vec{Y}| \, |\vec{Z}| \, (e^\varepsilon(\rho^\varepsilon) + \xi^\varepsilon(\rho^\varepsilon)) \end{aligned}$$

□

Proof of Proposition 3.3. Inequality (3.49) means that -assuming Theorem 3.4 holds- the last integral is non-positive in the limit $\varepsilon \to 0$ and one arrives at the inequality

$$\int_0^T \int_\Omega \vec{Y}^T \cdot (d\mu_{ij})_{ij} \vec{Z} \le \int_0^T \int_\Omega |\vec{Y}||\vec{Z}| d\mu \tag{3.50}$$

which means that the measures μ_{ij} are absolutely continuous with respect to μ. Then there exist μ-measurable functions ν_{ij} such that

$$d\mu_{ij}(x,t) = \nu_{ij}(x,t) d\mu(x,t).$$

Since the matrix $(\nu_{ij})_{ij}$ inherits the symmetry from (3.8), the matrix is positive semi-definite and by (3.50) it doesn't have eigenvalues ≥ 1, so that

$$0 \leq (\nu_{ij})_{ij} \leq \mathbf{id}\,.$$

This means there exists an orthonormal-basis $\vec{\nu}_i$ of eigenvectors with eigenvalues $\tilde{\lambda}_i \in [0,1]$ and one can write the matrix as

$$(\nu_{ij})_{ij} = \sum_{i=1}^{d} \tilde{\lambda}_i\, \vec{\nu}_i \otimes \vec{\nu}_i$$

where $\sum_i \vec{\nu}_i \otimes \vec{\nu}_i = \mathbf{id}$. For scalar functions $y \in C^0(\Omega \times [0,T])$ we have similarly

$$\int_0^T \int_\Omega y\, \varepsilon_k \underbrace{\mathrm{tr}(\nabla\rho^{\varepsilon_k} \otimes \nabla\rho^{\varepsilon_k})}_{=|\nabla\rho^{\varepsilon_k}|^2} = \int_0^T \int_\Omega y\,(e^{\varepsilon_k}(\rho^{\varepsilon_k}) + \xi^{\varepsilon_k}(\rho^{\varepsilon_k})) \tag{3.51}$$

and $\lim_{k\to\infty} \varepsilon_k \, \mathrm{tr}(\nabla\rho^{\varepsilon_k} \otimes \nabla\rho^{\varepsilon_k}) = \sum_i (\nu_{ii}) d\mu = \sum_i \tilde{\lambda}_i d\mu$. Recall that the trace of a matrix is the sum of its eigenvalues. Then (3.51) transfers to

$$\sum_i \tilde{\lambda}_i d\mu \leq d\mu,$$

i.e. $\sum_i \tilde{\lambda}_i \leq 1$.

Setting $\lambda_i := \tilde{\lambda}_i + \frac{1}{d-1}\left(1 - \sum_{j=1}^d \tilde{\lambda}_j\right) \in [0,1]$ we get

$$\mathbf{id} - (\nu_{ij})_{ij} = \mathbf{id} - \sum_i \tilde{\lambda}_i\, \vec{\nu}_i \otimes \vec{\nu}_i = \sum_i \lambda_i\,(\mathbf{id} - \vec{\nu}_i \otimes \vec{\nu}_i)\,.$$

Thus we set the limit varifold as

$$dV^t(x,P) = \sum_i \lambda_i(t,x)\, d\mu(t,x)\, \delta_{\vec{\nu}_i(t,x)}(P), \tag{3.52}$$

where $\delta_{\vec{\nu}_i}$ is the projection onto the hyperplane normal to $\vec{\nu}_i$.

□

By Proposition 3.15 we see that $V^t(.,.)$ is a varifold in the usual sense for almost every $t \geq 0$. Plugging (3.52) into the variation formula (2.4) and replacing the variables λ_i and $\vec{\nu}_i$ back we get for vector fields $X \in C_0^1(\Omega \times [0,T], \mathbb{R}^d)$

$$\begin{aligned}
\int_0^T \partial V^t(X)dt &= \int_0^T \int_{G(\Omega)} DX : P\, dV^t(x,P) \\
&= \int_0^T \int_\Omega \sum_i DX : [\mathbf{id} - \vec{\nu}_i(t,x) \otimes \vec{\nu}_i(t,x)]\, \lambda_i\, d\mu \\
&= \int_0^T \int_\Omega DX : [\mathbf{id} - (\nu_{ij})_{ij}]\, d\mu \\
&= \int_0^T \int_\Omega DX : [\mathbf{id}\, d\mu - (d\mu_{ij})_{ij}]\,.
\end{aligned}$$

3.2.8 Control of discrepancy measure

As we stated in our assumptions in Subsection 1.1 we incorporate homogeneous elasticity which gives the estimate

$$|W_{,\rho}(\rho, \mathcal{E}(\mathbf{u}))| \leq C(1 + |\rho| + |\mathcal{E}(\mathbf{u})|).$$

Then $W_{,\rho}(\rho^\varepsilon, \mathcal{E}(\mathbf{u}^\varepsilon))$ is in $L^2(\Omega)$ for almost all times $t > 0$, see Lemma 1.5. Note that Lemma 3.6 states the higher integrability of our concentration function ρ^ε.

So we can follow the proof of Chen in [Chen96] for the estimation of the discrepancy measure. We give all details on how to apply the elliptic theory and respective Sobolev embedding theory explicitly for dimensions ≤ 3. The proof is based on a blow-up technique for which we need some preparatory lemmas.

Lemma 3.18. *Assume $\varrho \in H^{1,2}_{loc}(\mathbb{R}^d)$ satisfies*

$$\Delta\varrho = \Psi'(\varrho). \tag{3.53}$$

Then ϱ is already $C^3(\mathbb{R}^d)$ and $-1 \leq \varrho \leq 1$ in $\mathbb{R}^d$ such that

$$|\nabla\varrho(x)|^2 \leq 2\Psi(\varrho(x)) \qquad \forall x \in \mathbb{R}^d \tag{3.54}$$

If equality holds in equation (3.54) in some point $x \in \mathbb{R}^d$, then equality holds everywhere and ϱ is either constant ± 1 or a planar wave.

Here ϱ being a planar wave means that there exist $\hat{x} \in \mathbb{R}^d$ and a unit vector $\vec{e} \in \mathbb{R}^d$ such that

$$\varrho(x) = q((x - \hat{x}) \cdot \vec{e}) \qquad \forall x \in \mathbb{R}^d,$$

where q solves the ODE

$$\ddot{q} = \Psi'(q), \quad q(0) = 0, \quad q(\pm\infty) = \pm 1. \tag{3.55}$$

There is a very similar statement which follows immediately from the above lemma by extension via reflection:

Lemma 3.19. *Assume $\varrho \in H^{1,2}_{loc}(\mathbb{R}^{d-1} \times [0, \infty))$ satisfies*

$$\Delta\varrho = \Psi'(\varrho) \quad \text{in } \mathbb{R}^{d-1} \times (0, \infty), \tag{3.56}$$

$$\tfrac{\partial}{\partial\nu}\varrho = 0 \quad \text{on } \mathbb{R}^{d-1} \times \{0\}. \tag{3.57}$$

Then ϱ is already $C^3(\mathbb{R}^{d-1} \times [0, \infty))$ and $-1 \leq \varrho \leq 1$ in $\mathbb{R}^{d-1} \times [0, \infty)$ such that

$$|\nabla\varrho(x)|^2 \leq 2\Psi(\varrho(x)) \qquad \forall x \in \mathbb{R}^{d-1} \times [0, \infty) \tag{3.58}$$

If equality holds in equation (3.54) in some point $x \in \mathbb{R}^{d-1} \times [0, \infty)$, then equality holds everywhere and ϱ is either constant ± 1 or a planar wave. In this case the wave has to be perpendicular to $\mathbb{R}^{d-1} \times \{0\}$.

Remark. Here we see that the 90° condition arises through the Neumann-boundary condition for ϱ.

Proof of Lemma 3.18.

(i) First we show that ϱ is a bounded C^3-function. We take a cut-off function $\zeta \in C^\infty(\mathbb{R}^d)$

$$0 \le \zeta \le 1, \quad \zeta = 1 \text{ in } B_{1/2}(0), \quad \zeta = 0 \text{ in } \mathbb{R}^d \setminus B_1(0). \tag{3.59}$$

Testing equation (3.53) with $\zeta^k \varrho$ with $k = 2p/(p-2)$ for $p > 2$ we can calculate

$$\begin{aligned} 0 &= \int \nabla\varrho \cdot \nabla(\zeta^k \varrho) - \Psi'(\varrho)\zeta^k \varrho \\ &= \int k\zeta^{k-1}\varrho\nabla\varrho \cdot \nabla\zeta + |\nabla\varrho|^2\zeta^k - \Psi'(\varrho)\zeta^k\varrho \end{aligned}$$

Using Young-inequality twice we can estimate the first summand by

$$\begin{aligned} \int k\zeta^{k-1}\varrho\nabla\varrho\cdot\nabla\zeta &= \int (\zeta^{k/2}\nabla\varrho)(k\zeta^{k/2-1}\varrho\nabla\zeta) \\ &\ge -1/2 \int \big((\zeta^k|\nabla\varrho|^2) + (k\zeta^{k-2}\varrho^2|\nabla\zeta|^2)\big) \\ &\ge -1/2 \int \big(\zeta^k|\nabla\varrho|^2 + \delta(k\,\zeta^{k-2}\varrho^2)^q + (C_\delta\, k\,|\nabla\zeta|^2)^{q'}\big). \end{aligned}$$

Choosing $q = p/2,\ q' = p/(p-2)$ yields the inequality

$$0 \ge \int \Big[|\nabla\varrho|^2\zeta^k - \Psi'(\varrho)\zeta^k\varrho - 1/2\left(\zeta^k|\nabla\varrho|^2 + \delta k^{p/2}\zeta^k\varrho^p + C_{\delta,p}k^{p/(p-2)}|\nabla\zeta|^k\right)\Big]. \tag{3.60}$$

Due to the form of Ψ (cf. Subsection 1.2) it holds for some $c_1, c_2 > 0$ that

$$r\Psi'(r) \ge c_1|r|^p - c_2 \qquad \forall r \in \mathbb{R}. \tag{3.61}$$

Then by choosing $\delta = \frac{c_1}{2k^{p/2}}$ the inequality (3.60) leads to

$$\int \zeta^k \left(|\nabla\varrho|^2 + |\varrho|^p\right) \le C(c_1, c_2, p, \|\nabla\zeta\|_k). \tag{3.62}$$

By changing the centre point of the cut-off function ζ to arbitrary $x_0 \in \mathbb{R}^d$, we arrive at a uniform bound $C > 0$:

$$\|\varrho\|_{H^{1,2}(B_{1/2}(x_0))} \le C \qquad \forall x_0 \in \mathbb{R}^d. \tag{3.63}$$

(ii) The right side of equation (3.53) is in $L^2(B_{1/2}(x_0))$ by the Sobolev embedding $H^{1,2}(B_{1/2}(x_0)) \hookrightarrow L^{2(p-1)}(B_{1/2}(x_0))$, so that ϱ is in fact in $H^{2,2}(B_{1/2}(x_0))$ by elliptic regularity theory. Now using the Sobolev embedding

$$H^{2,2}(B_{1/2}(x_0)) \hookrightarrow C^{0,\alpha}(B_{1/2}(x_0))$$

we get that the function ϱ, but then also $\Psi' \circ \varrho$ are bounded in the $L^\infty(B_{1/2}(x_0))$-norm and locally Hölder continuous. By applying elliptic theory for the linear Poisson equation, the solution ϱ is in $C^3(B_{1/4}(x_0))$ – more precisely, Proposition 10.1.2 by [Jos98] yields $C^2(B_{1/3}(x_0))$-regularity, then the right side of (3.53) is in $C^1(B_{1/3}(x_0))$ and Corollary 10.1.1 by [Jos98] concludes the desired $C^3(B_{1/4}(x_0))$-regularity.

By the uniform bound (3.63) which is independent of the centre point $x_0 \in \mathbb{R}^d$, the L^∞-bound and C^3-regularity extend uniformly to the whole space $\mathbb{R}^d$.

(iii) Now, we want to use a comparison principle like Theorem 10.1 of [GilTru98] to prove that in fact

$$|\varrho| \leq 1.$$

For any arbitrary $\delta > 0$ we take a connected subset Ω_δ of $\{x \in B_{1/\delta}(0) \mid \varrho(x) \geq 1 + \delta\}$ and show that it must be empty. With the comparison function

$$\varsigma(x) := 1 + \delta \exp\left(\delta_2 \sqrt{1 + |x|^2}\right) \tag{3.64}$$

we are going to use a comparison principle, as one can find in [GilTru98]. and further insight in [CrIshLi95].

For the quasi-linear operator Q defined as

$$Q(\varrho) := \Delta\varrho - \Psi'(\varrho) \tag{3.65}$$

we have to choose $\delta_2 > 0$ in such a way that $Q(\varrho) \geq Q(\varsigma)$ in Ω_δ. We calculate

$$\begin{aligned}\Delta\varsigma &= \delta\,\delta_2 \frac{\exp(\delta_2\sqrt{1+|x|^2})}{(\sqrt{1+|x|^2})^3}\left(\delta_2|x|^2\sqrt{1+|x|^2} + d + (d-1)|x|^2\right)\\ &\leq \delta\,\delta_2 \exp\left(\delta_2\sqrt{1+|x|^2}\right)(\delta_2 + d\sqrt{1+|x|^2})\end{aligned}$$

and on the other hand we have

$$\Psi'(\varsigma) \geq c_0\delta \quad \text{in } \Omega_\varepsilon \tag{3.66}$$

by the growth property of Ψ' for values greater than $1 + \delta$ (cf. definition (1.9)) and definition of ς (3.64). So, by an appropriate choice of δ_2 one can guarantee that

$$Q(\varsigma) \leq 0 = Q(\varrho) \quad \text{in } \Omega_\delta.$$

On the boundary we have on $\partial\Omega_\delta \cap B_{1/\delta}(0)$

$$\varrho \leq \varsigma,$$

which follows simply by construction of ς, and on $\partial\Omega_\delta \cap \partial B_{1/\delta}(0)$

$$\varsigma = 1 + \delta \exp\left(\delta_2\sqrt{1 + 1/\delta^2}\right)$$

which grows arbitrarily for small δ. So we can find a $\delta > 0$ such that

$$\varsigma \geq \|\varrho\|_\infty \quad \text{on } \partial\Omega_\delta \cap \partial B_{1/\delta}(0).$$

Then by above-mentioned comparison principle it follows that

$$\varrho \leq \varsigma \quad \text{in } \Omega_\delta.$$

Since $\delta > 0$ can be chosen arbitrarily small and we obtain

$$\varrho \leq 1.$$

With an analogue comparison using

$$\tilde{\varsigma}(x) := -1 - \delta \exp\left(\delta_2 \sqrt{1 + |x|^2}\right)$$

in order to get

$$\varrho \geq \tilde{\varsigma} \quad \text{in } \Omega_\delta,$$

we finally get

$$\|\varrho\|_\infty \leq 1.$$

(iv) Now it remains to show that estimate (3.54) holds and the case of the planar wave is true. Both follow from the work of Modica [Mod85], cited below, and its extension.

□

Theorem 3.20 (Modica, [Mod85])**.** *Let $F \in C^2(\mathbb{R})$ be a non-negative function and $\varrho \in C^3(\mathbb{R}^N)$ be a bounded solution in $\mathbb{R}^N, N \in \mathbb{N}$ of the nonlinear Poisson equation*

$$\Delta \varrho = F'(\varrho). \tag{3.67}$$

(i) Then

$$|\nabla \varrho|^2(x) \leq 2F(\varrho(x)) \quad \textit{for every } x \in \mathbb{R}^N. \tag{3.68}$$

(ii) If there exists a $x_0 \in \mathbb{R}^N$ such that $F(\varrho(x_0)) = 0$, then ϱ is already constant.

Proposition 3.21 (Extension to Modica's result)**.** *Moreover, if in the situation of the above theorem equality holds for (3.68) at some point $x_0 \in \mathbb{R}^N$ then equality holds everywhere. And if additionally $\varrho(x_0)$ is between two roots x_a, x_b of F, then the function ϱ is either constant or a planar wave.*

Remark. In the case that F has the additional property

$$\lim_{s \to \pm\infty} F(s) \geq C > 0,$$

ϱ cannot lie outside of all roots of F, if $|\nabla \varrho|^2 = 2F(\varrho)$.

Assume that $\varrho(x_0)$ does not lie between two roots of F, we can then construct a curve x_t starting in x_0 following the direction $\nabla \varrho(x_t)$. By continuation and for $|\nabla \varrho|^2 \equiv 2F(\varrho)$, the values $\varrho(x_t)$ increase beyond every limit. This is a contradiction to the assumption, therefore ϱ must be between two roots of F.

The function F plays the role of our potential Ψ.

Proof of Proposition 3.21. According to the theorem of Modica we know that the function

$$P := 1/2|\nabla\varrho|^2 - F(\varrho) \tag{3.69}$$

is non-positive. We now want to apply a maximum principle for P to show that P is in fact constant zero. Being a solution of the Poisson equation we get for ϱ that

$$\nabla P = \nabla\varrho^T D^2\varrho - F'\nabla\varrho, \qquad \Delta P = D^2\varrho : D^2\varrho - F'^2(\varrho).$$

On the other hand we have the estimate in every x

$$|\nabla\varrho|^2(D^2\varrho : D^2\varrho) \geq |D^2\varrho\nabla\varrho|^2 = |\nabla P + F'\nabla\varrho|^2 \geq 2F'\nabla P\cdot\nabla\varrho + F'^2|\nabla\varrho|^2.$$

If $|\nabla\varrho|(x_0) = 0$, then $F(\varrho(x_0)) = 0$ and by the second part of Modica's theorem ϱ is constant. Let us assume $|\nabla\varrho|(x_0) > 0$. Then we have (locally near x_0)

$$\Delta P - \frac{2F'\nabla P\cdot\nabla\varrho}{|\nabla\varrho|^2} \geq -F'^2 + F'^2 = 0. \tag{3.70}$$

If we modify the function F such that it is constant for values greater than $\|\varrho\|_{L^\infty}$, hence ϱ would still be a solution to equation (3.67), we then can apply the maximum principle A.5. In fact, we have recovered a quasilinear operator

$$Q = \Delta - 2\frac{F'}{|\nabla\varrho|^2}\nabla\varrho\cdot\nabla$$

such that $Q(P) \geq 0$. When applying Theorem A.5 note that P is non-positive by assumption and we choose Ω as the neighbourhood where (3.70) holds.

Since in our case we get that the function must be constant in the neighbourhood of x_0, by continuation the function P must be globally zero. Thus the first part of the proposition is proven.

Assume now that ϱ takes values strongly between two roots of F, say x_a, x_b. Let q be the unique solution of the ODE

$$\ddot{q} = F'(q), \qquad \text{with } q(0) = (x_a + x_b)/2,\ q(-\infty) = x_a,\ q(\infty) = x_b. \tag{3.71}$$

One can easily see that for q the derivative is $\dot{q} = \sqrt{2F(q)}$. Furthermore q is a strong monotonically increasing function, therefore injective and we can define uniquely a function z in $\mathbb{R}^N$ such that $\varrho(x) = q(z(x))$. The identity $|\nabla\varrho|^2 = 2F(\varrho)$ leads to $|\nabla z| = 1$ in $\mathbb{R}^N$, since we have also $\dot{q} = \sqrt{2F(q)}$. Plugging z into the Poisson equation, we get via

$$\Delta\varrho = \dot{q}\Delta z + \ddot{q}|\nabla z|^2 = \sqrt{2F}\Delta z + F'\,1$$

the Laplace equation

$$\Delta z = 0 \qquad \text{in } \mathbb{R}^N.$$

Again we can assume that $F \neq 0$ in any point $x \in \mathbb{R}^N$, since otherwise it is constant by the second part of Modica's result. We have already seen that z has linear growth, so the harmonic function has to be (affine) linear. This means that $\varrho = q \circ z$ is a planar wave. □

Lemma 3.22. *For each $\eta > 0$ there is a constant $R(\eta) > 2$ such that for all $R > R(\eta)$ the following holds:*

If

$$\hat{\Omega} = \{(x', x_d) \in B_R \mid x_d > Y(x')\}$$

is a domain in $\mathbb{R}^d$, $Y : \mathbb{R}^{d-1} \to \mathbb{R}$ satisfying

$$Y(0') \leq 0, \quad \nabla_{x'} Y(0') = 0', \quad \|D^2_{x'} Y\|_{C^0(B'_R)} \leq R^{-3} \tag{3.72}$$

and if $(\varrho, \mathbf{v}) \in H^{2,2}(\hat{\Omega}) \times L^2(\hat{\Omega})$ with

$$-\Delta\varrho + \Psi'(\varrho) = \mathbf{v} \qquad \text{in } \hat{\Omega}, \tag{3.73}$$

$$\tfrac{\partial}{\partial\nu}\varrho = 0 \qquad \text{on } \{(x', x_d) \in B_R \mid x_d = Y(x')\}, \tag{3.74}$$

$$\|\mathbf{v}\|_{L^2(B_R \cap \hat{\Omega})} \leq R^{-1}, \tag{3.75}$$

then the following inequality holds

$$\int_{B_1 \cap \hat{\Omega}} \left(|\nabla\varrho|^2 - 2\Psi(\varrho)\right)^+ \leq \eta \int_{B_2 \cap \hat{\Omega}} \left(|\nabla\varrho|^2 + \Psi'(\varrho)^2 + \Psi(\varrho) + \mathbf{v}^2\right) + \int_{\{x \in B_1 \cap \hat{\Omega} \mid |\varrho| \geq 1-\eta\}} |\nabla\varrho|^2. \tag{3.76}$$

Proof. We look closer on the interfacial region:

$$\hat{\Omega}^\eta_1 := \{x \in B_1(0) \cap \hat{\Omega} \mid |\varrho(x)| \leq 1 - \eta\}. \tag{3.77}$$

With $q := 2d/(d-2)$ for $d > 2$ and $q := 7$ for $d = 2$ and accordingly $m := 2q/(q-2)$, we consider the following two cases:

(i) For $|\hat{\Omega}^\eta_1| \leq \eta^m$ we get with Young-inequality and Sobolev embedding properties

$$\begin{aligned} \|\nabla\varrho\|_{L^2(\hat{\Omega}^\eta_1)} &\leq |\hat{\Omega}^\eta_1|^{\frac{q-2}{2q}} \|\nabla\varrho\|_{L^q(\hat{\Omega}^\eta_1)} \\ &\leq C\eta^{m/m} \|\nabla\varrho\|_{H^{1,2}(\hat{\Omega}^\eta_1)}. \end{aligned} \tag{3.78}$$

As the second derivatives are bounded through the Laplace-function we get

$$\begin{aligned} \|\nabla\varrho\|_{H^{1,2}(B_1(0)\cap\hat{\Omega})} &\leq C\left(\|\Delta\varrho\|_{L^2(B_2(0)\cap\hat{\Omega})} + \|\nabla\varrho\|_{L^2(B_2(0)\cap\hat{\Omega})}\right) \\ &\leq C\left(\|\mathbf{v}\|_{L^2(B_2(0)\cap\hat{\Omega})} + \|\Psi'\|_{L^2(B_2(0)\cap\hat{\Omega})} + \|\nabla\varrho\|_{L^2(B_2(0)\cap\hat{\Omega})}\right). \end{aligned} \tag{3.79}$$

Estimates (3.78) and (3.79) together yield

$$\|\nabla\varrho\|_{L^2(\hat{\Omega}^\eta_1)} \leq C\eta\left(\|\mathbf{v}\|_{L^2(B_2(0)\cap\hat{\Omega})} + \|\Psi'\|_{L^2(B_2(0)\cap\hat{\Omega})} + \|\nabla\varrho\|_{L^2(B_2(0)\cap\hat{\Omega})}\right)$$

which leads to

$$\int_{B_1(0)\cap\hat{\Omega}} |\nabla\varrho|^2 \leq C\eta^2 \int_{B_2(0)\cap\hat{\Omega}} \left(\mathbf{v}^2 + \Psi'^2 + |\nabla\varrho|^2\right) + \int_{\Omega^c_1} |\nabla\varrho|^2$$

where $\Omega^c_1 = \{x \in B_1(0) \cap \hat{\Omega} \mid |\varrho(x)| \geq 1 - \eta\}$.

(ii) For $|\hat{\Omega}_1^\eta| \geq \eta^m$ we are using a contradiction argument. Let's assume that the lemma is not true. Then we have a sequence $(\varrho^i, \mathbf{v}^i, \hat{\Omega}^i)_i$ such that for each $i \in \mathbb{N}$ the assumptions (3.75)-(3.72) of the lemma hold with $R = i$ and $|\tilde{\Omega}^i| := |\{x \in B_1(0) \cap \hat{\Omega}^i \mid |\varrho^i(x)| \leq 1 - \eta\}| \geq \eta^m$, but not estimate (3.76).

As in Lemma 3.18 we test our equation (3.73) with $\zeta^k \varrho^i$, see (3.59) for definition of ζ, to get

$$0 = \int \nabla \varrho^i \cdot \nabla(\zeta^k \varrho^i) - \Psi'(\varrho^i)\zeta^k \varrho^i - \mathbf{v}^i \zeta^k \varrho^i.$$

With the same calculation as in the proof of Lemma 3.18 and estimating the $\mathbf{v}^i$-term by

$$\begin{aligned}\int \mathbf{v}^i \zeta^k \varrho^i &\geq -\tfrac{1}{2} \int \zeta^k (\mathbf{v}^i)^2 + \zeta^k \rho^2 \\ &\geq -\tfrac{1}{2} \left(\int (\mathbf{v}^i)^2 + \delta \int \zeta^k (\rho^i)^p + C_\delta \int \zeta^k \right)\end{aligned}$$

altogether this results in

$$\int \zeta^k \left(|\nabla \varrho^i|^2 + |\varrho^i|^p \right) \leq C(c_1, c_2, p, \|\mathbf{v}^i\|_{L^2(\Omega)}, \|\nabla \zeta\|_k). \tag{3.80}$$

With the assumption

$$\|\mathbf{v}^i\|_{L^2(\Omega)} \leq C$$

we have the uniform bound

$$\|\varrho^i\|_{H^{1,2}(B_r \cap \Omega^i)} \leq C = C(r).$$

Using the Sobolev embedding $H^{1,2} \hookrightarrow L^q$ for some $q \geq 2$, such that equation (3.73) can be read as a linear Poisson equation with right side in L^2-, we have that ϱ^i is uniformly bounded in $H^{2,2}$:

$$\|\varrho^i\|_{H^{2,2}(B_r \cap \Omega^i)} + \|\Psi'(\varrho^i)\|_{L^2(B_r \cap \Omega^i)} \leq C = C(r). \tag{3.81}$$

Now, let Y^i be the function related to $\hat{\Omega}^i$. First, we assume that

$$\liminf_{j \to \infty} Y^j(0) = -\infty.$$

Then we can find a subsequence $(j^k)_k$ of $\mathbb{N}$ and a function $\varrho \in H^{2,2}_{\text{loc}}(\mathbb{R}^d)$ such that for $j^k \to \infty$ the following holds for arbitrary $r > 0$:

(i)	$Y^{j^k}(x') \to -\infty$	uniformly in compact subsets of $\mathbb{R}^{d-1}$,
(ii)	$\mathbf{v}^{j^k} \to 0$	in $L^2(B_r)$,
(iii)	$\varrho^{j^k} \to \varrho$	in $H^{1,2}(B_r)$ and in $C^{0,\alpha}(B_r)$,
(iv)	$\Psi'(\varrho^{j^k}) \to \Psi'(\varrho)$	in $L^q(B_r)$,
(v)	$-\Delta\varrho + \Psi'(\varrho) = 0$	in $H^{1,2}(B_r)$ and a.e. in $\mathbb{R}^d$.

ad (i): This follows from assumption (3.72). For large j^k the graph of Y^{j^k} is nearly flat.

ad (ii): This follows from assumption (3.75).

ad (iii): The above estimate (3.81) yields to compactness for the sequence ϱ^{j^k} in $H^{2,2}(B_r)$. That is, we have a weakly converging subsequence $\varrho^{j^k} \to \varrho$ to some $\varrho \in H^{2,2}(B_r)$. Using the compact embedding $H^{2,2}(B_r) \hookrightarrow C^{0,\alpha}(B_r)$ for dimension ≤ 3, ϱ^{j^k} is a locally uniformly converging sequence. Using the embedding into $H^{1,2}(B_r)$ the sequence also converges in $H^{1,2}$.

ad (iv): This follows by the above uniformly converging sequence $\varrho^{j^k} \to \varrho$.

ad (v): Combine the above convergences $(ii), (iii)$ and (iv).

Now, we can apply Lemma 3.18 which gives

$$\lim_{k\to\infty} \int_{B_1} \left(|\nabla \varrho^{j^k}|^2 - 2\Psi(\varrho^{j^k}) \right)^+ = \int_{B_1} \left(|\nabla \varrho|^2 - 2\Psi(\varrho) \right)^+ = 0. \qquad (*)$$

At the same time the right side of (3.76) is uniformly positive (in j^k). For large j we get

$$\left|\{x \in B_1 \mid |\varrho^j| \leq 1 - \eta\}\right| = \left|\tilde{\Omega}^j\right| \geq \eta^m,$$

since by part (i) the graph of Y^j moves to minus infinity and $\hat{\Omega}^j \cap B_1$ becomes B_1. But then with the pointwise convergence of $\varrho^j \to \varrho$ we get

$$\lim_{k\to\infty} \eta \int_{B_1} \left|\nabla \varrho^j\right|^2 + \Psi(\varrho^j) = \eta \int_{B_1} |\nabla \varrho|^2 + \Psi(\varrho) \geq \eta\, \eta^m \min_{s\in[-1+\eta,1-\eta]} \Psi(s). \quad (**)$$

From $(*)$ and $(**)$ we get a contradiction, as the right side of $(**)$ is positive, independent from k.

In the case

$$\mathbf{y} := \liminf_{j\to\infty} Y^j(0) > -\infty$$

we have $Y^j \to \mathbf{y}$ uniformly in $B_r(0)$ for all $r > 0$. This again follows from assumption (3.72), since Y^j becomes more and more flat. Analogue convergences of ϱ^j as in the upper case hold in $B_r(0) \cap \{x \mid x_d > \mathbf{y}\}$. Then the contradiction results from applying Lemma 3.19.

□

Now we need a control on the bulk energy of the interface. This is shown in the following lemma.

Lemma 3.23. *There exist positive constants C_0 and η_0 such that for every $\eta \in (0, \eta_0]$, every $\varepsilon \in (0, 1]$ and every $(\rho, v) \in \mathcal{K}_\varepsilon$ the following holds*

$$\int_{\{x\in\Omega \mid |\rho|\geq 1-\eta\}} \left(e^\varepsilon(\rho) + \tfrac{1}{\varepsilon}\Psi'(\rho)^2\right) \leq C_0\eta \int_{\{x\in\Omega \mid |\rho|\leq 1-\eta\}} \varepsilon|\nabla\rho|^2 + C_0\varepsilon \int_\Omega v^2. \qquad (3.82)$$

Proof. Let $\eta \in (0, c_0/2)$ with c_0 from (1.10). We are using the convexity property (1.10) of our potential for values $|\rho| \geq 1-\eta$. Define a function g by

$$g(s) := \begin{cases} \Psi'(s) & \text{for } |s| \geq 1-\eta \\ 0 & \text{for } |s| \leq 1-c_0 \end{cases} \tag{3.83}$$

and in between linear. Now, on one side we have

$$\int_\Omega vg(\rho) = \int_\Omega \big(\varepsilon g'(\rho)|\nabla\rho|^2 + \tfrac{1}{\varepsilon}\Psi'(\rho)g(\rho)\big),$$

but using $\big|\int_\Omega vg(\rho)\big| \leq \int_\Omega (\frac{\varepsilon}{2}v^2 + \frac{1}{2\varepsilon}g^2) \leq \int_\Omega (\frac{\varepsilon}{2}v^2 + \frac{1}{2\varepsilon}\Psi'\, g)$, we get

$$\begin{aligned}
&\int_{\Omega\cap\{|\rho|\geq 1-\eta\}} \left(\varepsilon\Psi''(\rho)|\nabla\rho|^2 + \frac{1}{\varepsilon}\Psi'^2(\rho)\right) \\
&\quad = \int_{\Omega\cap\{|\rho|\geq 1-\eta\}} \left(\varepsilon g'(\rho)|\nabla\rho|^2 + \frac{1}{\varepsilon}\Psi'(\rho)g(\rho)\right) \\
&\quad \leq \int_\Omega \left(\frac{\varepsilon}{2}v^2 + \frac{1}{2\varepsilon}\Psi'(\rho)g(\rho)\right) - \int_{\Omega\cap\{|\rho|\leq 1-\eta\}} \big(\varepsilon g'(\rho)|\nabla\rho|^2 + \tfrac{1}{\varepsilon}\Psi'(\rho)g(\rho)\big) \\
&\quad \leq \int_\Omega \frac{\varepsilon}{2}v^2 - \int_{\Omega\cap\{|\rho|\leq 1-\eta\}} \varepsilon g'(\rho)|\nabla\rho|^2 \\
&\qquad - \int_{\Omega\cap\{|\rho|\geq 1-\eta\}} \frac{1}{2\varepsilon}\Psi'(\rho)g(\rho) + \int_{\Omega\cap\{|\rho|\geq 1-\eta\}} \frac{1}{2\varepsilon}\Psi'(\rho)g(\rho).
\end{aligned}$$

Now, moving the last term to the left side (note that in this case $\Psi' = g$) and using $\Psi'\, g \geq 0$ we have overall

$$\begin{aligned}
&\int_{\Omega\cap\{|\rho|\geq 1-\eta\}} \left(\varepsilon\Psi''(\rho)|\nabla\rho|^2 + \frac{1}{\varepsilon}\Psi'^2(\rho)\right) \\
&\qquad \leq \frac{\varepsilon}{2}\int_\Omega v - \int_{\Omega\cap\{|\rho|\leq 1-\eta\}} \varepsilon g'(\rho)|\nabla\rho|^2.
\end{aligned}$$

Since the function g is a linear extension of

$$g(1-c_0) = 0 \quad \text{and} \quad g(1-\eta) = \Psi'(1-\eta)$$

in the interval $(0, 1-\eta)$ (and analogue for negative values), the derivative is simply zero or

$$\left|g'\left(\tfrac{(1-c_0)+(1-\eta)}{2}\right)\right| = \big|\Psi'(1-\eta)/(c_0-\eta)\big| \leq \big|2\Psi'(1-\eta)/c_0\big| \leq C\eta.$$

The last inequality is due to the structure of Ψ' which has simple root in ± 1 (the tangent of $\Psi'(\pm 1)$ intersects the real axis). To complete the proof we use that for $|s| \geq 1-c_0$ the potential Ψ is convex according to (1.9), moreover is fulfils

$$\Psi'' \geq c_0|x|^{p-2} \geq c_0|1-\eta|^{p-2} = C > 0$$

plus we have the estimate $\Psi(r) \leq C\Psi'(r)^2$ for $|r| \geq 1-c_0$. □

Now, we are ready to proof Theorem 3.4:

Proof of Theorem 3.4. Let $(\rho, v) \in \mathcal{K}_\varepsilon$. We choose $\eta > 0$ arbitrary small, $R(\eta)$ as in Lemma 3.22 and $\varepsilon = 1/R \in (0, R(\eta)^{-2})$, more precisely given below. Now we choose a maximal set $\{x_j \mid j \in \mathcal{T}\}$ satisfying

$$\inf_{i \neq j} |x_i - x_j| \geq \varepsilon.$$

Then clearly $\{B_\varepsilon(x_j)\}_{j \in \mathcal{T}}$ is a covering of Ω which in fact satisfies

$$\sum_{j \in \mathcal{T}} \chi_{B_{2\varepsilon}(x_j) \cap \Omega} \leq C(n) \quad \text{and} \quad \sum_{j \in \mathcal{T}} \chi_{B_{2R}(x_j) \cap \Omega} \leq C(n) R^d. \tag{3.84}$$

Remark. We assume additionally that $\varepsilon > 0$ is small enough that each ball $B_\varepsilon(x_j)$ is simply connected, so we don't run into problems when doing the blow-up (cf. properties of the graph function Y^j of the boundary).

For each $j \in \mathcal{T}$ we define the rescaled functions

$$\begin{cases} \varrho^j(y) & := \rho^\varepsilon(x_j + \varepsilon y) \\ \mathbf{v}^j(y) & := \varepsilon\, v^\varepsilon(x_j + \varepsilon y) \end{cases} \qquad \text{for } y \in \Omega^j := \{y \mid x_j + \varepsilon y \in \Omega\}. \tag{3.85}$$

Then these functions solve the equation

$$-\Delta_y \varrho^j + \Psi'(\varrho^j) = \mathbf{v}^j \tag{3.86}$$

in $B_R(x_j) \cap \Omega^j$. The important point is now to observe that the boundary of the original domain Ω is scaled by $1/\varepsilon$ through this blow-up, so that for $j \in \mathcal{T}$ with $\partial\Omega^j \cap B_R(x_j) \neq \emptyset$ we can (possibly after a rotation) describe the boundary part of $\partial\Omega^j \cap B_R(x_j)$ by a function $Y \colon \mathbb{R}^{d-1} \to \mathbb{R}$ with

$$Y(0') \leq 0,\ D_{y'} Y(0') = 0 \ \text{ and } \ \|D^2_{y'} Y\|_{C^0(B'_R)} \leq C \|\partial\Omega\|_{C^2} \varepsilon^2. \tag{3.87}$$

Now, $\varepsilon > 0$ is chosen in such a way that assumption (3.72) of Lemma 3.22 holds for each $j \in \mathcal{T}$ with $R = 1/\varepsilon$.

We divide the set of indices $\mathcal{T} := \mathcal{A} \dot\cup \mathcal{B}$ by

$$\begin{aligned} \mathcal{A} &= \{j \in \mathcal{T} \mid \|v^\varepsilon\|_{L^2(B_{R\varepsilon}(x_j) \cap \Omega)} \leq \varepsilon^{d/2-1} R^{-1}\}, \\ \mathcal{B} = \mathcal{T} \setminus \mathcal{A} &= \{j \in \mathcal{T} \mid \|v^\varepsilon\|_{L^2(B_{R\varepsilon}(x_j) \cap \Omega)} > \varepsilon^{d/2-1} R^{-1}\}. \end{aligned}$$

case $j \in \mathcal{A}$: Since for the rescaled function $\mathbf{v}^j$ we have by transformation rules

$$\|\mathbf{v}^j\|_{L^2(B_R(0) \cap \Omega^j)} = \varepsilon^{-d/2} \|\varepsilon v^\varepsilon\|_{L^2(B_{R\varepsilon}(x_j) \cap \Omega)} \leq R^{-1},$$

we can apply Lemma 3.22 and get

$$\begin{aligned} \int_{B_1(0) \cap \Omega^j} \left(|\nabla \varrho^j|^2 - 2\Psi(\varrho^j)\right)^+ &\leq \eta \int_{B_2(0) \cap \Omega^j} \left(|\nabla \varrho^j|^2 + \Psi(\varrho^j) + \Psi'^2(\varrho^j) + (\mathbf{v}^j)^2\right) \\ &\quad + \int_{B_1(0) \cap \{y \in \Omega^j \,|\, |\varrho^j(y)| \geq 1 - \eta\}} |\nabla \varrho^j|^2. \end{aligned}$$

Reversing the blow-up this inequality becomes

$$\int_{\Omega^j} (\xi^\varepsilon(\rho^\varepsilon))^+ \leq \eta \int_{B_{2\varepsilon}(x_j)\cap\Omega} \Big(e^\varepsilon(\rho^\varepsilon) + \varepsilon^{-1}{\Psi'}^2(\rho^\varepsilon) + \varepsilon(v^\varepsilon)^2 \Big) + \int_{B_{2\varepsilon}(x_j)\cap\{y\in\Omega||\rho^\varepsilon(y)|\geq 1-\eta\}} \varepsilon|\nabla\rho^\varepsilon|^2.$$

Summing up all $j \in \mathcal{A}$ gives

$$\sum_{j\in\mathcal{A}} \int_{\Omega^j} (\xi^\varepsilon(\rho^\varepsilon))^+ \leq \eta\, C \int_\Omega \big(e^\varepsilon(\rho^\varepsilon) + \varepsilon(v^\varepsilon)^2 \big) + \eta\, C \int_{\{y\in\Omega||\rho^\varepsilon(y)|\leq 1-\eta\}} \varepsilon^{-1}{\Psi'}^2(\rho^\varepsilon) + C \int_{\{y\in\Omega||\rho^\varepsilon(y)|\geq 1-\eta\}} \varepsilon|\nabla\rho^\varepsilon|^2 + \varepsilon^{-1}{\Psi'}^2(\rho^\varepsilon).$$

Using Lemma 3.23 on the third integral results in

$$\sum_{j\in\mathcal{A}} \int_{\Omega^j} \big(\xi^\varepsilon(\rho^j)\big)^+ \leq \eta\, C \int_\Omega e^\varepsilon(\rho^\varepsilon) + \varepsilon\, C \int_\Omega (v^\varepsilon)^2, \tag{3.88}$$

where we used that for $|s| \leq 1$ we have $(\Psi')^2 \leq C\Psi$, so that

$$\int_{\{y\in\Omega||\rho^\varepsilon(y)|\leq 1-\eta\}} \varepsilon^{-1}{\Psi'}^2(\rho^\varepsilon) \leq C \int_\Omega \varepsilon^{-1}\Psi(\rho^\varepsilon) \leq C \int_\Omega e^\varepsilon(\rho^\varepsilon).$$

case $j \in \mathcal{B}$**:** For the second case, we simply estimate the full $\int |\nabla\rho|^2$-term. To get an elliptic estimates similar to (3.80) we test (3.86) with $\zeta^2\varrho^j$, ζ as in (3.59) for $B_1 \subset B_2$.

$$\begin{aligned} 0 &= \int \nabla\varrho^j \cdot (\zeta^2\varrho^j) - \Psi'(\varrho^j)\zeta^2\varrho^j - \mathbf{v}^j\zeta^2\varrho^j \\ &\geq \int \Big[\big(|\nabla\varrho^j|^2\zeta^2 - \tfrac{1}{2}|\nabla\varrho^j|^2\zeta^2 - 2|\nabla\zeta|^2(\varrho^j)^2\big) \\ &\qquad - \big((\Psi'(\varrho^j))^2 + (\varrho^j)^2\big) - \big((\mathbf{v}^j)^2 + (\varrho^j)^2\big) \Big]. \end{aligned}$$

This gives the estimate

$$\int_{B_1} \left|\nabla\varrho^j\right|^2 \leq C \int_{B_2\cap\Omega^j} \Big({\Psi'}^2(\varrho^j) + |\mathbf{v}^j|^2 + |\varrho^j|^2 \Big)$$

and using $|\varrho^j|^2 \leq C((\Psi'(\varrho^j))^2 + 1)$ and $\Psi'(r) \leq C$ for $|r| \leq 1$ we get

$$\int_{B_1} \left|\nabla\varrho^j\right|^2 \leq C + C \int_{B_2} |\mathbf{v}^j|^2 + {\Psi'}^2(\varrho^j)\chi_{\{|\varrho^j|\geq 1\}}.$$

Again we reverse to blow-up and sum over all $j \in \mathcal{B}$ to get

$$\sum_{j\in\mathcal{B}} \int_{\Omega^j} \varepsilon|\nabla\rho^\varepsilon|^2 \le C\varepsilon^{-1} \sum_{j\in\mathcal{B}} |B^j| + C\varepsilon \int_\Omega v^{\varepsilon 2} + C\varepsilon^{-1} \int_{\{x\in\Omega||\rho^\varepsilon(x)|\ge 1\}} \Psi'^2$$
$$\le C\varepsilon^{-1} \sum_{j\in\mathcal{B}} |B^j| + C\varepsilon \int_\Omega v^{\varepsilon 2} \tag{3.89}$$

where the second inequality follows from Lemma 3.23 with $\eta = 0$. Now using $j \in \mathcal{B}$

$$\int_{B_{R\varepsilon}(x_j)\cap\Omega} v^{\varepsilon 2} \ge R^{-2}\varepsilon^{d-2} \ge \varepsilon^{-2}R^{-2}|B^j|/|B_1|$$

it follows that

$$\sum_{j\in\mathcal{B}} |B^j| \le \varepsilon^2|B_1|R^2 \sum_{j\in\mathcal{B}} \int_{B_{R\varepsilon}(x_j)} v^{\varepsilon 2} \le \varepsilon^2|B_1|R^2CR^d \int_\Omega v^{\varepsilon 2}. \tag{3.90}$$

Plugging this estimate into (3.89), we obtain

$$\sum_{j\in\mathcal{B}} \int_{B^j} \varepsilon|\nabla\rho^\varepsilon|^2 \le C(1+R^{d+2})\varepsilon \int_\Omega v^{\varepsilon 2}. \tag{3.91}$$

This yields to the estimate for $\Omega_{\mathcal{B}} := \Omega \cap (\cup_{j\in\mathcal{B}} B^j)$

$$\int_{\Omega_{\mathcal{B}}} (\xi^\varepsilon(\rho^\varepsilon))^+ = \int_{\Omega_{\mathcal{B}}} \left(\tfrac{\varepsilon}{2}|\nabla\rho^\varepsilon|^2 - \tfrac{1}{\varepsilon}\Psi(\rho^\varepsilon)\right)^+ \le \int_{\Omega_{\mathcal{B}}} (\tfrac{\varepsilon}{2}|\nabla\rho^\varepsilon|^2)^+ \overset{(3.91)}{\le} C\,\varepsilon \int_\Omega v^{\varepsilon 2}, \tag{3.92}$$

since Ψ is non-negative.

Combining estimate (3.88) with (3.92) we finally get

$$\int_\Omega (\xi^\varepsilon(\rho^\varepsilon))^+ \le C\eta \int_\Omega e^\varepsilon(\rho^\varepsilon) + \varepsilon M(\eta) \int_\Omega v^{\varepsilon 2}.$$

□

Proof of Theorem 3.5. We now have to go through points (i) to (v) of Definition 3.1 and verify the conditions for our limit functions and measures.

(i) The diffusion equation follows directly from the stated convergences of proposition 3.2.

(ii) On one hand we have the variation of our varifold given by equation (3.10), and on the other we have a variant of the Gibbs-Thomson law in equation (3.48). Using the almost-everywhere in time result of Proposition 3.15, we can indeed localise the equations, because there are no time derivatives of the test-functions involved.

(iii) In Lemma 3.9 we derived the convergence of the Modica modification of the concentration function $\tilde{\rho}^\varepsilon$. In fact by the previous Lemma 3.8 we have a compactness in $BV(A)$ for any subset $A \subset \Omega$, so that by the weak lower semi-continuity of the norm in $BV(A)$ we get

$$\begin{aligned}2\sigma \int_t^\tau |D\chi_{M^s}|(A) ds &\leq \liminf_{\varepsilon \to 0} \int_t^\tau \int_A |\nabla \tilde{\rho}^\varepsilon| dx\, ds \\ &= \liminf_{\varepsilon \to 0} \int_t^\tau \int_A \sqrt{2\tilde{\Psi}(\rho^\varepsilon)} |\nabla \rho^\varepsilon| dx\, ds \\ &\leq \liminf_{\varepsilon \to 0} \int_t^\tau \int_A e^\varepsilon dx\, ds \\ &= \int_t^\tau \int_A d\mu(s,x).\end{aligned}$$

For the first equality recall Lemma 3.7. Now we can look at the pointwise behaviour in space and time of the measures $D\chi_{M^s}$ and $\mu(s,x)$ and using Proposition 3.15 we have for almost every time and almost every $x \in \Omega$ the stated inequality.

(iv) This is part of Lemma 3.16.

(v) This is an immediate consequence of equation (3.3) in the limit $\varepsilon \to 0$ and considering the strong $L^2(\Omega)$ convergence of ρ^ε and strong $H^{1,2}(\Omega)$ convergence of the deformation vector $\mathbf{u}^\varepsilon$.

□

3.2.9 Rectifiability issue

We are going to show that the varifold which is derived in the previous subsections is for almost every time $t \in [0, T]$ a rectifiable varifold, if one adds one further assumption on the density of the varifold:

$$\limsup_{r \to 0} \frac{1}{r^{d-1}} \mu_{V^t}(B_r(x_0)) \geq \theta \tag{3.93}$$

for some $\theta > 0$ for μ_{V^t}-almost every x. More precisely this would mean that the varifold is a measure on a countably $(d-1)$-rectifiable set with a locally $\mathcal{H}^{d-1}$-integrable weight function, see Definition 2.6. First we cite a result from [Gar00] about a higher integrability of the deformation vector:

Theorem 3.24 (Higher integrability). *There exists a $s_\bullet \in (2, p)$ such that for all $\mathbf{v} \in H^{1,2}(\Omega, \mathbb{R}^d)$ which fulfil for all $\eta \in H^{1,2}(\Omega, \mathbb{R}^d)$ the identity*

$$\int_\Omega W_{,\mathcal{E}}(\rho, \mathcal{E}(\mathbf{v})) : \nabla \eta = 0, \tag{3.94}$$

where ρ is bounded in $L^p(\Omega)$, the integrability property

$$\nabla \mathbf{v} \in L^{s_\bullet}(\Omega, \mathbb{R}^{d\times d})$$

holds. Moreover,

$$\|\nabla \mathbf{v}\|_{L^{s_\bullet}(\Omega,\mathbb{R}^{d\times d})} \leq C(\|\nabla \mathbf{v}\|_{L^2(\Omega,\mathbb{R}^{d\times d})} + \|\rho\|_{L^p(\Omega)} + 1)$$

with C independent of ρ.

We can apply this theorem to the pointwise in time variant of equation (v) in Definition 3.1 for our limit deformation vector function $\mathbf{u}(t,.)$ and set $\rho = -1 + 2\chi_{M^t}$. Then by the above theorem

$$\nabla \mathbf{u}(t,.) \in L^{s_\bullet}(\Omega, \mathbb{R}^{d\times d})$$

for some $s_\bullet \in (2,p)$. If we now look at the description of the first variation of our varifold (ii) in Definition 3.1, then the first variation of the varifold is a dual element on $\mathring{H}^{1,s_\bullet/2}(\Omega,\mathbb{R}^d)$ by the estimates

$$\left|\int_\Omega \chi_{M^t} \operatorname{div}(wY)\right| \leq C\|w\|_{H^{1,2}(\Omega)}\|Y\|_{H^{1,2}(\Omega)}, \tag{3.95}$$

$$\left|\int_\Omega \mathrm{Esh} : DY\right| \leq C\|\mathrm{Esh}\|_{L^s(\Omega)}\|DY\|_{L^{s^*}(\Omega)} \tag{3.96}$$

for $Y \in C_0^1(\Omega)$ where $s := s_\bullet/2$, $s^* := s/(s-1)$ and $\mathrm{Esh} := \big(W\,\mathbf{id} - (\nabla\mathbf{u})^T S\big)$ is the Eshelby tensor. Combining the two estimates we get

$$|\langle \partial V, Y\rangle| \leq C\|Y\|_{H^{1,s^*}(\Omega)}, \tag{3.97}$$

i.e. $\partial V \in \big(\mathring{H}^{1,s}(\Omega,\mathbb{R}^d)\big)^* = \mathring{H}^{1,s^*}(\Omega,\mathbb{R}^d)$. On $\mathring{H}^{1,s^*}(\Omega,\mathbb{R}^d)$ we have a representative A in $L^s(\Omega,\mathbb{R}^{d\times d})$ for the varifold which fulfils

$$\langle \partial V, Y\rangle = \int_\Omega A : DY. \tag{3.98}$$

If we now define

- $\mu_1(A) := \int_A |\mathrm{Esh}|\,dx$,
- $\mu_2(A) := \int_A |\mathrm{Esh}|^s\,dx$,
- $F(r,L) := Cr^{1/s^*}L^{1/s}$

with C as in (3.97), then the function $g(L) := \inf_{R\geq 0}(F(R,L) + R^{-d+1})$ has the estimate

$$\begin{aligned} g(L) &\leq F(L^{-1/(ds-1)}, L) + L^{(d-1)/(ds-1)} \\ &\leq C(L^{-1/(s^*(ds-1))}L^{1/s} + L^{(d-1)/(ds-1)}) \\ &\leq CL^{(d-1)/(ds-1)}. \end{aligned}$$

As $s > 1$ the last exponent $(d-1)/(ds-1)$ is smaller than 1, therefore

$$\lim_{L\to\infty} \frac{g(L)}{L} = 0.$$

This means we can apply the rectifiability result by Luckhaus 2.14.

It is easy to see that condition (3.93) holds for all $x \in \partial M^t$, but for the phantom interface $\mathrm{supp}(\mu_{V^t}) \setminus \partial M^t$ no such density estimate is known a priori. Using Allard's theorem 2.10 the restriction onto the set

$$\{x \in \Omega \mid \theta^{*d-1}(\mu_{V^t}, x) > 0\} \tag{3.99}$$

is rectifiable.

3.3 Related results

In the comparison study of models of phase separating phenomena including elastic misfit there have been published some results so far. In Section 1.2 we already mentioned the Γ-limit property of the respective energy functionals by Garcke, see [Gar00]. This means that minimisers of the phase-field model converge to a minimiser of the sharp interface model. The papers by Fried and Gurtin, see [FrGu94], and Jou, Leo and Lowengrub, see [JLL98], were the first ones to relate the two models. They used matched asymptotic expansions for which one has to assume that there exists a smooth solution of the sharp interface problem. Further numerical results emphasised the relation, see [GLNRW06] and references therein. The present work now proves rigorously the relation of the time-dependent models.

The following works do not cover the phase separating phenomena including elastic misfit, but are closely related by techniques or results.

Tonegawa has extensively analysed the asymptotical behaviour of phase-field equations in several articles, as in [Ton03] and in collaboration with Hutchinson [HutTon00] and recently with Röger [RögTon07]. Tonegawa (representatively speaking inclusively for his co-authors as well) looked on time-dependent Allen-Cahn equations, see [Ton03], and the stationary Cahn-Hilliard equations, [RögTon07] and [HutTon00]. One helpful assumption for the initial phase-field functions were uniform bounds besides to energy bounds. So one may simplify the main results of his work as

> If one has phase-field solutions with certain additional properties (i.e. bounds), *then* they converge to some sharp-interface varifold solution with a suitable Gibbs-Thomson law.

In our case we want to use established existence theory for the phase-field equations, so that we only have to specify the initial data and derive the resulting solution functions by those existence statements, which unfortunately do not give any bounds except energy estimates. Nevertheless we proof the converging behaviour of these phase-field functions to a generalised sharp-interface solution.

The L^∞-bound from [HutTon00] would be also helpful in our case, the time-dependent Cahn-Hilliard system including elastic effects, but our aim was different from his work, as we wanted to start off with phase-field functions given by the existence theory at hand. In other words we only choose suitable initial data and the main message of our analysis is that we have a provable asymptotic behaviour in the time-space continuum.

In the papers by Brakke, [Bra78], Luckhaus and Sturzenhecker, [LuStu95], and Almgren, Taylor and Wang, [AlTaWa93], the solutions of the mean curvature flow equation are studied. Here they don't deal with an asymptotic limit, but they develop the existence of a solution by incorporating a time discretisation method for the sharp-interface model. Therefore phase-field functions do not occur here as when studying asymptotic limits.

One important source of this work is the paper by Chen [Chen96]. He studied the asymptotic limit of the Cahn-Hilliard model. Chen showed for arbitrary spatial dimensions that solutions of the Cahn-Hilliard system converge globally in time to some generalised sharp-interface solution. He could not prove that the limit varifold is rectifiable, but in the case $p = 2$, $d = 3$ one can use the Theorem 2.11 by Schätzle to deduce rectifiability for the limit varifold of the Cahn-Hilliard systems without elasticity on the set where the mass measure of the varifold has positive $(d-1)$-dimensional density: In the case of Cahn-Hilliard systems, i.e. without any elastic terms, equation (ii) in Definition 3.1 becomes of the same form as in the Theorem 2.11 by Schätzle. This means that one can deduce rectifiability of the varifold in the case without elasticity, at least for the case $d \leq 3$ with the same restriction as in (3.99).

There is one significant difference to results for the related Allen-Cahn models which are proposed to describe motion of phase boundaries driven by surface tension:

$$\varepsilon \frac{\partial \rho}{\partial t} = \varepsilon \Delta \rho - \tfrac{1}{\varepsilon} \Psi'(\rho).$$

As Ilmanen [Ilm93] has studied the limit behaviour of the Allen-Cahn equation towards the mean curvature flow in the sense of Brakke [Bra78], he confirmed that one gets in the limit

$$\lim_{\varepsilon \to 0} \xi^\varepsilon = 0.$$

This is also known as *equi-partition of energy*. It is interesting to see that the interface energy is asymptotically equally distributed between the $|\nabla \rho^\varepsilon|^2$- and the $\Psi(\rho^\varepsilon)$-part. Moreover this result can be used for further results, namely it is easier to deduce the fact that the resulting interface varifold is rectifiable. This is much stronger than in the Cahn-Hilliard and Cahn-Larché case, where only the inequality

$$\lim_{\varepsilon \to 0} \xi^\varepsilon \leq 0$$

can be achieved.

After Ilmanen [Ilm93] first used geometric measure theory to prove such convergence in $\Omega = \mathbb{R}^d$, Soner [Son95] improved the result for more general settings. Hutchinson and Tonegawa studied in [HutTon00] the asymptotic behaviour of critical, not necessarily minimal points of the Cahn-Hilliard energy functional. In their work they also used geometric measure theory and derived local estimates for the discrepancy measure (3.5). By that, they gained convergence results for bounded domains. In their (time-independent) setting the limit varifold turns out to be integral, i.e. the interface has indeed integer multiplicity modulo a surface constant almost everywhere. Moreover local minimisers of the Cahn-Hilliard energy functional converge to a local area minimiser subject to a volume constraint. Later Tonegawa extended with similar estimates the results by Ilmanen and showed that time-dependent solutions of the Allen-Cahn equation converge to an integral varifold solution of the mean curvature flow, cf. [Ton03].

4 Examples

In this chapter we want to analyse the dynamics of simple cases. The goal is to see which parameters mostly determine the behaviour of the system. The cases are described in the sharp-interface model language which has been proposed in the first chapter.

4.1 One dimensional case

If we observe an interval which is simply divided into two subintervals of distinct phases, we know that the interface of this system will not have any motion, as the mass of each phase is preserved and we deny in our analysis any mass exchange across the boundary.

So, for possibly non-trivial dynamics of an elastical system, we need at least two interfaces.

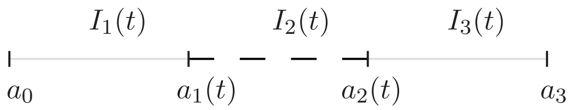

Figure 5: 1-dimensional case

We look at the interval $I = [a_0, a_3]$ divided into three subintervals by $a_0 < a_1 < a_2 < a_3$. The two outer subintervals represent the phase $\oplus$, the inner one $\ominus$. Then the equations (1.19)–(1.22) turn into

$$
\begin{aligned}
w'' &= 0 && \text{in } I_k(t), && (4.1)\\
V &= 1/2[w']_-^+ && \text{in } a_l(t), && (4.2)\\
w &= 1/2[W - \mathbf{u}'S]_-^+ && \text{in } a_l(t), && (4.3)\\
\mathbf{u}'' &= 0 && \text{in } I_k(t), && (4.4)\\
[S] = [\mathbf{u}] &= [w] = 0 && \text{in } a_l(t) && (4.5)
\end{aligned}
$$

for $k = 1, 2, 3$ and $l = 1, 2$ together with homogeneous Neumann boundary conditions for $S, \mathbf{u}$ and w. Note that V denotes the normal velocity in direction from the phase $\oplus$ to the phase $\ominus$. Equation (4.4) originates from the divergence-free stress tensor for one dimension.

In our ansatz we assume the elastic energy to have the form

$$
\begin{aligned}
W^{\pm} &= W^{\pm}(\mathbf{u}') = \tfrac{1}{2}\mathcal{C}^{\pm}(\mathbf{u}' - \mathcal{E}_{\pm}^{*})^2, && (4.6)\\
S^{\pm} &= S^{\pm}(\mathbf{u}') = \mathcal{C}^{\pm}(\mathbf{u}' - \mathcal{E}_{\pm}^{*}), && (4.7)
\end{aligned}
$$

where $\mathcal{C}^{\pm}$ is the respective elasticity tensor to the phases $\oplus$ and $\ominus$ and $\mathcal{E}_{\pm}^{*}$ the corresponding eigenstrain.

By equation (4.4) the deformation function $\mathbf{u}$ is assumed to be of the form

$$\mathbf{u}(x) = \alpha_k x + \beta_k \quad \text{in } I_k \text{ for } k = 1, 2, 3. \qquad (4.8)$$

Then the Gibbs-Thomson law (4.3) transforms to

$$w = 1/2 \begin{cases} (\alpha_0 + \mathcal{E}_+^*)\mathcal{C}^+(\alpha_0 + \mathcal{E}_+^*) - (\alpha_1 + \mathcal{E}_-^*)\mathcal{C}^-(\alpha_1 + \mathcal{E}_-^*) & \text{in } a_1(t) \\ (\alpha_2 + \mathcal{E}_+^*)\mathcal{C}^+(\alpha_2 + \mathcal{E}_+^*) - (\alpha_1 + \mathcal{E}_-^*)\mathcal{C}^-(\alpha_1 + \mathcal{E}_-^*) & \text{in } a_2(t). \end{cases} \tag{4.9}$$

The chemical potential has to fulfil

$$w'' = 0 \tag{4.10}$$

in each of the subintervals which we denote by I_1, I_2 and I_3. Furthermore w has to be continuous, so altogether it is a piecewise linear function, as was the deformation function $\mathbf{u}$. If we assume homogeneous Neumann boundary conditions, w is constant on I_1 and I_3. Then by (4.2) we see that the interface will move according to the slope of w in the middle interval I_2. More precisely we have the motion law:

$$\dot{a}_1(t) = -w_1'(a_1(t)) \tag{4.11}$$

$$\dot{a}_2(t) = -w_1'(a_2(t)) \tag{4.12}$$

which follows from equation (4.2).

The slope of w is determined by the values of w at the interfaces, which follows by the Gibbs-Thomson law. In the one-dimensional case there is no curvature term. So, the elastic system determines the chemical potential.

If the system is in a thermo-dynamical equilibrium, i.e. equations (4.5) hold, then this essentially means that the interfaces do not move. In short, the continuity of the deformation function and stress tensor yield that the slopes of the deformation function in the $\oplus$-phase coincide:

$$\alpha_0 = \alpha_2 \tag{4.13}$$

and from (4.9) the potential function w has the same value in both $a_1(t)$ and $a_2(t)$, meaning

$$w \equiv const \qquad \text{in the whole } I.$$

The crucial point is that in the one-dimensional case the Eshelby-tensor (the right hand side of (4.3)) does not depend on $x \in I$. Moreover the mechanical equilibrium forces the values of w to coincide in $a_1(t)$ and $a_2(t)$ according to (4.9).

Remark. By similar calculations the case with arbitrarily many interfaces is stable, if Neumann boundary conditions hold. Then again, the slopes of the deformation function of the respective phases coincide as in equation (4.13).

4.1.1 Non-equilibrium

Since in the equilibrium 1-dimensional case, we have seen that there is no dynamics of the interfaces, we examine now the case of the *inhomogeneous Neumann-Problem:*

Imposing a force from outside is described by some fixed boundary values for the stress tensor

$$S^+(a_0) := S_0^*, \qquad S^+(a_3) := S_3^*. \tag{4.14}$$

If

$$S_0^* = -S_3^*,$$

then one can calculate that this leads again to an equilibrium state, thus we don't have any dynamics of the interfaces. Note that this case corresponds to the existence of a function $\tilde{\mathbf{u}}$ with

$$S_0^* = S(\tilde{\mathbf{u}})(a_0), \quad S_3^* = S(\tilde{\mathbf{u}})(a_3).$$

In the other case

$$S_0^* \neq -S_3^*,$$

a mechanical equilibrium cannot be reached. But this in fact leads to a difference in (4.9) and the potential w is not constant in I any more. By the boundary condition (4.14) the values for the deformation function by (4.8) attain

$$\alpha_1 = -S_0^*, \qquad \alpha_3 = S_3^*.$$

We don't actually need to specify any of the other parameters, especially values for $\mathbf{u}|_{I_2(t)}$, as the motion law (4.11) and (4.12) depend only on the slope of w, i.e. in this case only on the difference of the Eshelby-tensor. The difference of the Eshelby-tensor according to (4.9) does not change by the slope of $\mathbf{u}$ in the middle interval I_2, since α_1 cancels out. So, altogether the boundary conditions (4.14) determine the motion of the interfaces and switching the values S_0^* and S_3^* will simply invert the behaviour.

It is furthermore remarkable that the velocity of the interface-movement does not vary, i.e. we see a uniform speed of the interface throughout the observation phase.

4.1.2 Energy

One way to explain the stability is to refer to the underlying energy of our system:

$$\mathbf{E} = \sigma \sharp\{\text{interfaces}\} + \int_{I_1 \cup I_3} W^+ + \int_{I_2} W^- \tag{4.15}$$

$$= \sigma \sharp\{\text{interfaces}\} + W^+(|I_1| + |I_3|) + W^- |I_2| \,. \tag{4.16}$$

The last equality follows, as the elastic energy does not vary within one phase, cf. definitions (4.6) and (4.8). Note that the length of the intervals $I_1 \cup I_3 = I^\oplus$, respectively $I_2 = I^\ominus$, is fixed by the conservation of mass. Therefore the elastic energy fraction does not change at all. So, the only way to decrease the energy is by reducing the number of interfaces. But this cannot be done continuously. Looking at the energy landscape the energy is constant in a neighbourhood of our initial data. Then the time evolution which follows the steepest descent has no direction to follow, cf. the discussion of gradient-flows in Section 1.3 – moreover the evolution of the sharp-interface model has a gradient-flow structure, as it is discussed in [GLNRW06].

In the non-equilibrium case we see that the indecisiveness of the gradient flow is overcome by enforcing stress from outside. In the non-equilibrium case the energy landscape is still locally constant around our initial state. So the gradient flow structure wouldn't suggest any motion. Anyway the outer stress overcomes this steadiness.

For the behaviour of the non-equilibrium case above we observe that the energy stays constant over time, until one of the interfaces touches the outer boundary and the system looses one interface. At this point the energy drops by one unit of interface energy σ.

4.2 Rotation-symmetric case

Like in one dimension, we need at least two interfaces to observe some dynamics in the rotation-symmetric case for dimensions $d \geq 2$. This case gets a bit more complicated than the one-dimensional one. We start with new notations:

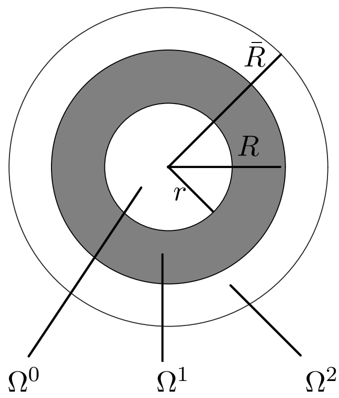

Figure 6: Rotation-symmetric case

We take $\Omega = B_{\bar{R}}(0) \subset \mathbb{R}^d$ as the domain under observation. In the symmetric case all subdomains are assumed to be concentric to the origin: Let

$$\Omega^0 := B_r(0), \qquad \Omega^1 := B_R(0) \setminus \overline{B_r(0)}, \qquad \Omega^2 := B_{\bar{R}}(0) \setminus \overline{B_R(0)}$$

be the initial three phases, the middle one representing phase $\ominus$, the other two phase $\oplus$ and

$$\Gamma^0 := \partial B_r(0), \qquad \Gamma^1 := \partial B_R(0), \qquad 0 < r < R < \bar{R}$$

the two interfaces of our system.

We are interested in the motion of the interfaces, so we denote by

$$\Omega^k(t),\ \Gamma^l(t)$$

for $k = 0, 1, 2$ and $l = 0, 1$ the time-dependent partition of $\bar{\Omega}$. We mark functions with an upper index k as the restrictions to $\Omega^k(t)$.

The underlying equations are

$$\Delta \bar{w}^k = 0, \qquad \text{in } \Omega^k(t), \tag{4.17}$$

$$V_{\Gamma^l(t)} = 1/2[\nabla \bar{w}]_-^+ \nu, \qquad \text{on } \Gamma^l(t), \tag{4.18}$$

$$\bar{w} = \sigma\kappa + 1/2\, \nu \cdot \left[W - \nabla \bar{\mathbf{u}}^T S\right]_-^+ \nu, \qquad \text{on } \Gamma^l(t), \tag{4.19}$$

where $\bar{w}$ is the potential function, V the normal velocity of the interface, W the elastic energy density, $\bar{\mathbf{u}}$ the deformation vector and $S = W_{,\mathcal{E}}$ the stress tensor, ν the normal pointing into the phase $\oplus$. We assume the functions to depend only on the radius and the elastic energy density to be of the quadratic form

$$\bar{w}(x,t) = w(|x|,t), \quad \bar{\mathbf{u}}(x,t) = \mathbf{u}(|x|,t)\tfrac{x}{|x|}, \quad W^{\pm}(\mathcal{E}) = \tfrac{1}{2}\left(\mathcal{E} - \bar{\mathcal{E}}^{\pm}\right) : \mathcal{C}^{\pm}\left(\mathcal{E} - \bar{\mathcal{E}}^{\pm}\right). \tag{4.20}$$

Here $\mathcal{C}^{\pm}$ is the elasticity tensor of the respective phase and

$$\bar{\mathcal{E}}^{\pm} = q^{\pm}\,\mathbf{id}$$

the respective eigenstrain tensor. For w and $\mathbf{u}$ we impose homogeneous Neumann boundary conditions

$$\partial_\nu w = \partial_\nu \mathbf{u} = 0, \tag{4.21}$$

but regarding the stress tensor we consider inhomogeneous Neumann boundary conditions to observe outer mechanical forces

$$\mathcal{C}^+(\mathcal{E}(\nabla\mathbf{u}) - \bar{\mathcal{E}}^+)\underbrace{\nu}_{=\frac{x}{|x|}} = S^*\nu = s^*\,\mathbf{id}\,\tfrac{x}{|x|}. \tag{4.22}$$

Note that in the rotation symmetric case the strain tensor is simply the gradient of the deformation vector:

$$\mathcal{E}(\mathbf{u}) = 1/2\left(\nabla\mathbf{u} + \nabla\mathbf{u}^T\right) = \nabla\mathbf{u}.$$

On the interfaces w, $\mathbf{u}$ and $S\nu$ are supposed to be continuous:

$$\mathbf{u}^0(r(t),t) = \mathbf{u}^1(r(t),t), \quad \mathcal{C}^+(\mathcal{E}(\mathbf{u}^0) - \bar{\mathcal{E}}^+)x = \mathcal{C}^-(\mathcal{E}(\mathbf{u}^1) - \bar{\mathcal{E}}^-)x \;\text{ on } \partial B_{r(t)}(0), \tag{4.23}$$

$$\mathbf{u}^1(R(t),t) = \mathbf{u}^2(R(t),t), \quad \mathcal{C}^-(\mathcal{E}(\mathbf{u}^1) - \bar{\mathcal{E}}^-)x = \mathcal{C}^+(\mathcal{E}(\mathbf{u}^2) - \bar{\mathcal{E}}^+)x \;\text{ on } \partial B_{R(t)}(0). \tag{4.24}$$

The mechanical equilibrium translates to

$$\operatorname{div}\, \mathcal{C}^+(\mathcal{E}(\mathbf{u}^{0,2}) - \bar{\mathcal{E}}^+) = \operatorname{div}\, \mathcal{C}^+(\mathcal{E}(\mathbf{u}^{0,2})) = 0, \qquad \text{in } \Omega^0 \cup \Omega^2, \tag{4.25}$$

$$\operatorname{div}\, \mathcal{C}^-(\mathcal{E}(\mathbf{u}^1) - \bar{\mathcal{E}}^-) = \operatorname{div}\, \mathcal{C}^-(\mathcal{E}(\mathbf{u}^1)) = 0, \qquad \text{in } \Omega^1. \tag{4.26}$$

In the rotation-symmetric case the Laplace equation (4.17) for $\bar{w}$ changes to

$$\Delta\bar{w} = \frac{1}{r^{d-1}}\frac{\partial}{\partial r}\left(r^{d-1}\frac{\partial w}{\partial r}\right) = 0.$$

Then we can integrate the equation with respect to r:

$$r^{d-1}\frac{\partial w}{\partial r} = c_1$$

and solve the resulting ordinary differential equation of first order:

$$\frac{\partial w}{\partial r} = c_1 r^{1-d} \quad \Longrightarrow \quad w = \begin{cases} \omega_1 \ln(r) + \omega_2, & \text{for } d = 2, \\ -\omega_1 r^{2-d} + \omega_2, & \text{for } d \geq 3. \end{cases} \tag{4.27}$$

By the outer boundary condition for the chemical potential according to (4.21), w^2 has to be constant. w^0 also has to be constant, since otherwise we get a singularity in 0 and the resulting function is not in $H^{1,2}(\Omega^0(t))$. This means that w is only non-constant in $\Omega^1(t)$ and which is determined by the Gibbs-Thomson law

$$w = \hat{w}_0 := \frac{-d\,\sigma}{r(t)} + \frac{x}{|x|} \cdot \left[W\,\mathbf{id} - (\nabla \mathbf{u}^T)S\right]_-^+ \frac{x}{|x|} \qquad \text{on } \Gamma^0(t), \tag{4.28}$$

$$w = \hat{w}_2 := \frac{d\,\sigma}{R(t)} + \frac{x}{|x|} \cdot \left[W\,\mathbf{id} - (\nabla \mathbf{u}^T)S\right]_-^+ \frac{x}{|x|} \qquad \text{on } \Gamma^1(t). \tag{4.29}$$

In the rotation-symmetric case, the mean curvature turns out to be d-times the inverse of the curvature. The sign of the curvature changes as the respective normal vector is pointing inwards for Γ^0 and pointing outwards for Γ^1. σ denotes the surface energy density. With $w^0 \equiv w^2 \equiv 0$ the motion law (4.18) simplifies to

$$V_{\Gamma^0(t)} = 1/2\,\nabla \bar{w}^1 \cdot \frac{x}{|x|} \qquad V_{\Gamma^1(t)} = -1/2\,\nabla \bar{w}^1 \cdot \frac{x}{|x|} \tag{4.30}$$

$$= -1/2\,(w^1)'(r(t)), \qquad = -1/2\,(w^1)'(R(t)), \tag{4.31}$$

which translates to

$$\dot{r}(t) = -1/2\,(w^1)'(r(t)), \qquad \dot{R}(t) = -1/2\,(w^1)'(R(t)). \tag{4.32}$$

Once we calculate the values $\hat{w}_0$ and $\hat{w}_2$ from (4.28) and (4.29), we can easily compute the velocities of the interfaces by using (4.27):

$d = 2$**:** The values ω_1 and ω_2 are given by

$$\omega_1 \ln(r) + \omega_2 = \hat{w}_0, \qquad \omega_1 \ln(R) + \omega_2 = \hat{w}_2.$$

So we get

$$\omega_1 = \frac{\hat{w}_2 - \hat{w}_0}{\ln(R) - \ln(r)}, \qquad \omega_2 = \hat{w}_2 - \frac{\hat{w}_2 - \hat{w}_0}{\ln(R) - \ln(r)},$$

which results into

$$\dot{r}(t) = -1/2\,\nabla w \cdot \frac{x}{|x|} = \frac{-\omega_1}{2r^2} x \cdot \frac{x}{|x|} = (\hat{w}_0 - \hat{w}_2)\,\frac{1}{2r(\ln(R) - \ln(r))}. \tag{4.33}$$

$d \geq 3$: Here the values ω_1 and ω_2 are given by

$$\frac{\omega_1}{r^{d-2}} + \omega_2 = \hat{w}_0, \qquad \frac{\omega_1}{R^{d-2}} + \omega_2 = \hat{w}_2.$$

So we get

$$\omega_1 = \frac{\hat{w}_2 - \hat{w}_0}{R^{2-d} - r^{2-d}}, \qquad \omega_2 = \hat{w}_2 - \frac{\hat{w}_2 - \hat{w}_0}{R^{d-2}(R^{2-d} - r^{2-d})},$$

which results into

$$\dot{r}(t) = -1/2\, \nabla w \cdot \frac{x}{|x|} = \frac{(d-2)\omega_1}{2\, r^d} x \cdot \frac{x}{|x|} = (\hat{w}_0 - \hat{w}_2)\, \frac{R^{d-2}(d-2)}{2\, r(R^{d-2} - r^{d-2})}. \quad (4.34)$$

By equations (4.33) and (4.34), we see that for all dimensions $d \geq 2$ it is the sign of the difference $(\hat{w}_0 - \hat{w}_2)$ that indicates the growth or shrinking of the inner phase and by conservation of mass therefore also the respective behaviour of the outer interface.

4.2.1 The elasticity system

We want to express the elastic deformation function explicitly by material parameters and the underlying geometry. We follow the ansatz $\bar{\mathbf{u}}(x) = \mathbf{u}(|x|)\frac{x}{|x|}$ from (4.20), so the strain tensor simplifies to

$$\mathcal{E}(\mathbf{u})(x) = \nabla \bar{\mathbf{u}}(x) = \mathbf{u}'(|x|)\tfrac{x}{|x|}$$

and we use the assumption that the elasticity tensor is described by the so-called Lamé-constants E, ν, see [Brae91] for more information.

$$\mathcal{C}^{\pm}\, \mathcal{E} = \frac{E^{\pm}}{1+\nu^{\pm}}\, \mathcal{E} + \frac{E^{\pm}\nu^{\pm}}{(1+\nu^{\pm})(1-2\nu^{\pm})}\, \operatorname{tr} \mathcal{E}\ \mathbf{id} \quad (4.35)$$

where $E^{\pm}$ is the respective elasticity module and $\nu^{\pm}$ the respective Poisson number of each phase. Note that only certain ranges of Lamé-constants are admissible:

$$E^{\pm} \geq 0, \quad \nu^{\pm} \in (0, 1/2). \quad (4.36)$$

Then the stress tensor becomes (neglecting $\pm$ for the following calculations - both cases are the same)

$$\begin{aligned} S + \mathcal{C}\,\bar{\mathcal{E}} = \mathcal{C}\,\mathcal{E}(\mathbf{u}) &= \frac{E}{(1+\nu)}\mathcal{E} + \frac{E\nu}{(1+\nu)(1-2\nu)} \operatorname{tr} \mathcal{E}\, \mathbf{id} \\ &= \frac{E}{1+\nu}\,\frac{\mathbf{u}'(\tau)}{\tau} x \otimes x + \frac{E}{1+\nu}\mathbf{u}(\tau)\, \mathbf{id} + \frac{E\nu}{(1+\nu)(1-2\nu)} \big(\mathbf{u}'(\tau)\tau + d\mathbf{u}(\tau)\big)\, \mathbf{id}\,. \end{aligned}$$

We can calculate the divergence of the stress tensor as

$$\begin{aligned}
\nabla\cdot S &= \frac{E}{1+\nu}\nabla\cdot\Big(\frac{\mathbf{u}'(\tau)}{\tau}x\otimes x\Big) + \frac{E}{1+\nu}\mathbf{u}'(\tau)\frac{x}{|x|} \\
&\quad + \frac{E\nu}{(1+\nu)(1-2\nu)}\Big(\mathbf{u}''(\tau)\tau\frac{x}{|x|} + \mathbf{u}'(\tau)\frac{x}{|x|} + d\mathbf{u}'(\tau)\frac{x}{|x|}\Big) \\
&= \frac{E}{1+\nu}\Big(\frac{\mathbf{u}'(\tau)}{\tau}d + \mathbf{u}''(\tau)\Big)x + \frac{E}{1+\nu}\mathbf{u}'(\tau)\frac{x}{|x|} \\
&= \frac{E(1-\nu)}{(1+\nu)(1-2\nu)}\Big(\frac{\mathbf{u}'(\tau)}{\tau}(d+1) + \mathbf{u}''(\tau)\Big)x,
\end{aligned}$$

since

$$\begin{aligned}
\nabla\cdot\Big(\frac{\mathbf{u}'(\tau)}{\tau}x\otimes x\Big) &= \Big(\sum_j \partial_j\big(\frac{\mathbf{u}'(\tau)}{\tau}x_i x_j\big)\Big)_i \\
&= \Big(\sum_j \Big(\frac{\mathbf{u}'(\tau)}{\tau}(\delta_{ij}x_j + x_i) + \frac{\mathbf{u}''(\tau)}{\tau}\frac{x_j}{\tau}x_i x_j - \frac{\mathbf{u}'(\tau)}{\tau^2}\frac{x_j}{\tau}x_i x_j\Big)\Big)_i \\
&= \Big(\frac{\mathbf{u}'(\tau)}{\tau}(d+1)x_i + \frac{\mathbf{u}''(\tau)}{\tau^2}x_i\tau^2 - \frac{\mathbf{u}'(\tau)}{\tau^2}\frac{\tau^2}{\tau}x_i\Big)_i \\
&= \Big(\frac{\mathbf{u}'(\tau)}{\tau}d + \mathbf{u}''(\tau)\Big)x.
\end{aligned}$$

So, equations (4.25) and (4.26) become

$$\begin{aligned}
& 0 = \nabla\cdot S \\
\Leftrightarrow\quad & 0 = \Big(\frac{\mathbf{u}'(\tau)}{\tau}(d+1) + \mathbf{u}''(\tau)\Big) = \tau^{-(d+1)}\big(\mathbf{u}'(\tau)\tau^{d+1}\big)' \\
\Leftrightarrow\quad & \upsilon_1 = \mathbf{u}'(\tau)\tau^{d+1}.
\end{aligned}$$

This means that the deformation function has the form

$$\mathbf{u}(\tau) = \upsilon_1 + \upsilon_2\,\tau^{-d}, \tag{4.37}$$

more precisely we have in each region

$$\mathbf{u}^0(\tau) = \upsilon_1^0 + \upsilon_2^0\,\tau^{-d} \quad \text{in } \Omega^0, \tag{4.38}$$

$$\mathbf{u}^1(\tau) = \upsilon_1^1 + \upsilon_2^1\,\tau^{-d} \quad \text{in } \Omega^1, \tag{4.39}$$

$$\mathbf{u}^2(\tau) = \upsilon_1^2 + \upsilon_2^2\,\tau^{-d} \quad \text{in } \Omega^2. \tag{4.40}$$

The coefficients $\upsilon_1^k, \upsilon_2^k$ are determined by the continuity conditions

$$\mathbf{u}^0(r(t)) = \mathbf{u}^1(r(t)), \qquad S^0(\mathcal{E}(\mathbf{u}^0(r(t)))) = S^1(\mathcal{E}(\mathbf{u}^1(r(t)))), \tag{4.41}$$

$$\mathbf{u}^1(R(t)) = \mathbf{u}^2(R(t)), \qquad S^1(\mathcal{E}(\mathbf{u}^1(R(t)))) = S^2(\mathcal{E}(\mathbf{u}^2(R(t)))), \tag{4.42}$$

and the boundary condition

$$S^2(\mathcal{E}(\mathbf{u}^2(\bar{R})))\nu = S^*\nu. \tag{4.43}$$

If $\upsilon_2^0 \neq 0$, then $\mathbf{u}$ has a singularity in zero and we can exclude this case. This means that five parameters υ_l^k remain to determine the function $\mathbf{u}$ which are given by the equations (4.41)-(4.43). See appendix A.2 for the calculations.

Eigenstrains in the rotation-symmetric case can only have the form

$$\bar{\mathcal{E}} = q\,\mathbf{id} \tag{4.44}$$

with q some real number. We denote $q^{\pm}$ as the scalar eigenstrain for the $\oplus/\ominus$-phases respectively.

4.2.2 Case studies

We look on some cases of variables based on the calculations in appendix A.2. Basically we want to know the sign of $V_{\Gamma^0(t)}$ which will tell us, if the inner particle will shrink or grow. Up to a positive constant the result is a complicated quotient, see A.2 and confer remarks to (4.33) and (4.34). We remind of the constraint for admissible Lamé-constants (4.36) and note the additional inequalities

$$\sigma > 0, \quad d \geq 2, \quad 0 < r < R < \bar{R}$$

which follow from our ansatz. As it has been proposed in [Brae91] we assume for simplicity $\nu^+ = \nu^- = 1/3$. We use the notation $E := E^+/E^-$.

If $V_{\Gamma^0(t)}$ is positive, then the inner particle will shrink. As explained in equation (4.34), it is sufficient to look at $(\hat{w}_2 - \hat{w}_0)$. From (4.33) and (4.34) we see that a positive sign of $(\hat{w}_2 - \hat{w}_0)$ means a shrinking inner particle.

The denominator is

$$\begin{aligned}
&24E^+rR\big((d-1)(E-1)(d-1+(d+1)E)R^d(R^d-r^d)\\
&\quad+((d^2-1)(E-1)^2r^d-(1+d+(d-1)E)(-1+d+(d+1)E)R^d)\bar{R}^d\big)^2\\
&\qquad= 24E^+rR\Big(\big[-(d-1)^2-2(d-1)E+(d^2-1)E^2\big]R^d(R^d-r^d)\\
&+\big[-(d^2-1)(R^d-r^d)+2((1-d^2)r^d-(d^2+1)R^d)E-(d^2-1)(R^d-r^d)E^2\big]\bar{R}^d\Big)^2.
\end{aligned}$$

It is strictly positive for all admissible choices of parameters, if one has a look on the coefficients with respect to powers of $E = E^+/E^-$. This means we only need to find out the sign of the numerator, which is unfortunately more complicated. We consider following cases.

(i) The case $\sigma \gg 0$: This means that the surface energy becomes very large. As we can see from the Gibbs-Thomson law (4.19), the motion becomes similar to the non-elastic case for large surface energy σ. It is then clear that the inner phase always decreases, since it has a stronger curved boundary and the mass of the phase $\ominus$ diffuses from the inner to the outer region.

(ii) The case $E^+ = E^-$ which is equivalent to $E = 1$: This case is also unambiguous. We get

$$(\hat{w}_2 - \hat{w}_0) = \frac{3(d-1)(1+d)^2 E^-(q^+ - q^-)^2(R^d - r^d)rR + 16(R+r)\sigma d^2 R^2}{16drR^{d+1}} > 0$$

which means that if the elasticity modules coincide, then the inner particle always shrinks. Especially for the homogeneous case where the elasticity tensors coincide this result applies. This is different from the related mean curvature flow with elastic misfit, see [GaNüSt07].

(iii) The case $S^* \gg 0$: If we look at the coefficient of the highest order term (which is two) of S^*, then this will determine the case for very large S^*. The coefficient

$$16(d-1)d^2(E-1)^2 rR(R^d - r^d)\bar{R}^{2d} \cdot \\ \cdot \Big((3d - 3 + (2+12d)E)R^d + (3d + 3 + (4d-2)E)r^d + (1+d)E^2(R^d - r^d)\Big)$$

is strictly positive considering the admissible parameters (4.36). Here, the inner particle will shrink. Note that this is the case both for negative and positive large S^*, as the term is of quadratic order in S^*. This means that in the case of large outer forces it doesn't depend on whether we squeeze or pull.

(iv) The case $E \sim 0$ (i.e. $E^+ \ll E^-$): The nominator reduces to

$$48(d-1)^2 drR(R^d - r^d)^2 \bar{R}^{2d} S^{*2}$$

which is strictly positive. Again the inner particle will shrink.

(v) The case $E^+ \gg E^-$: This is the case when the inner and outer part is much "harder" than the middle part. The nominator becomes

$$(d-1)(d+1)rR(R^d - r^d)^2 \bar{R}^d [3(d+1)E^-(q-1)q^- - 4S^*] \cdot \\ \cdot \Big[3(d+1)E^-(q-1)q^-(2(\bar{R}^d - R^d) - d(\bar{R}^d - 2R^d)) - 4d\bar{R}^d S^*\Big].$$

The first terms in front of the brackets are all positive and we can simplify the two brackets by

$$[A_1 - 4S^*][A_1 A_2 - 4A_3 S^*]$$

using $A_1 = 3(d+1)E^-(q-1)q^-$, $A_2 = 2(\bar{R}^d - R^d) - d(\bar{R}^d - 2R^d)$, $A_3 = d\bar{R}^d$. So we have a non-degenerate quadratic polynomial in S^* which has the roots

$$S_1^* = \frac{A_1 A_2}{4A_3}, \qquad S_2^* = \frac{A_1}{4}.$$

One can easily verify that

$$A_2 = A_3 \quad \Leftrightarrow \quad \bar{R} = R,$$

so that the roots are different. But this means that $(S_1^*, S_2^*) \subset \mathbb{R}$ is a non-degenerate interval and for outer given stress values S^* between the roots S_1^* and S_2^* the nominator can become negative, the inner particle will actually grow.

(vi) The case $S^* = 0$: For the last case we consider no boundary stress. In two dimensions the nominator becomes

$$(r+R)\Big(27E^+(q^- - q^+)^2(R-r)rR^3\bar{R}^2\big[16E\bar{R}^2 + (E-1)(1+3E)(R-r)(r+R)\big] \\ +4\big((E-1)(1+3E)R^2(R^2-r^2) + (3(E-1)^2r^2 - (3+E)(1+3E)R^2)\bar{R}^2\big)^2\sigma\Big)$$

Here we see again that the second sum (the last line) including the surface energy σ has a positive factor, so it is overall positive. Nevertheless the first term can turn negative for $E \sim 0$ due to the $(E-1)$ factor inside the brackets. If then additionally σ is very small, the overall evolution lets the inner particle grow.

The three dimensional case is slightly different, as the nominator becomes

$$3\Big(3EE^-(q^- - q^+)^2(R^3 - r^3)rR\bar{R}^3 \\ \big[4(E-1)(1+2E)R^3(R^3-r^3) + ((E-1)(1+2E)r^3 + (1+(37-2E)E)R^3)\bar{R}^3\big] \\ +2(r+R)\big[(E-1)(1+2E)R^3(R^3-r^3) + (2(E-1)^2r^3 - (2+E)(1+2E)R^3)\bar{R}^3\big]^2\sigma\Big).$$

As in the 2-dimensional case the factor of the σ-term is positive. If E is very small and R larger than one fourth of $\bar{R}$, then the term in the brackets becomes negative.

If one models the case of large elastic forces by setting the surface energy σ small, by the above observation we have pointed out possible combinations of materials where in the rotation-symmetric case the inner particle does not necessarily shrink as in the non-elastic case. Note that in comparison to the work of [GaNüSt07] we have to observe three regions at least, compared to sufficient two regions in the case of mean curvature flow and its elastic modification in the mentioned paper. There are some slightly different results regarding the “elastic feature” that the inner particle might not necessarily vanish in finite time.

A Appendix

A.1 Cited Results

Here we gather general results about functional analysis, partial differential equation theory and probability and measure theory.

Theorem A.1 (Arzela-Ascoli Theorem)**.** *Let F be a Banach space and E a compact metric space. Then the set $H \subset C^0(E,F)$ is relatively compact, if and only if*

(i) H is equi-continuous and

(ii) for all $x \in E$ the set $H(x) := \{f(x) \mid f \in H\} \subset F$ is relatively compact.

Proof. See [Dieu60]. □

Theorem A.2 (Embedding Theorem)**.** *Let Y be a Banach space and $I \subset \mathbb{R}^d$ a compact set. Then the embedding $C^\alpha(I,Y) \to C^{\alpha'}(I,Y)$ is compact for $0 < \alpha' < \alpha < 1$.*

Remark. In the application in Subsection 3.2.3 we take $I = [0,T]$ and $Y = L^1(\Omega)$.

Proof. This follows from the analogue version found in [Alt02], using the extended version of Arzela-Ascoli theorem A.1. □

Theorem A.3 (Korn's inequality)**.** *For $\Omega \subset \mathbb{R}^d$ bounded and open with Lipschitz boundary, there exists a constant $c > 0$ such that*

$$\int_\Omega \mathcal{E}(\mathbf{u}) : \mathcal{E}(\mathbf{u}) \geq c\|\mathbf{u}\|_{H^{1,2}(\Omega)} \quad \forall\, \mathbf{u} \in \mathrm{X}_{\mathrm{ird}}^{\perp} \tag{A.1}$$

where

$$\begin{aligned} \mathrm{X}_{\mathrm{ird}} := \{\mathbf{u} \in H^{1,2}(\Omega,\mathbb{R}^d) | \ &\textit{there exist } b \in \mathbb{R}^d \textit{ and a skew symmetric} \\ &A \in \mathbb{R}^{d\times d} \textit{ such that } \mathbf{u}(x) = b + Ax\} \\ = \{\mathbf{u} \in H^{1,2}(\Omega,\mathbb{R}^d) \mid \ &\mathcal{E}(\mathbf{u}) = 0\} \end{aligned}$$

Proof. See [Zei88]. □

Proposition A.4. *Let $u \in H^{1,2}(\Omega)$ be a weak solution of the Poisson equation*

$$-\Delta u = f \qquad \textit{in } \Omega, \tag{A.2}$$

$$\partial_\nu u = 0 \qquad \textit{on } \partial\Omega \tag{A.3}$$

$$\textit{and} \quad \int_\Omega u = 0. \tag{A.4}$$

for a function $f \in C^1(\bar\Omega)$ with $\int_\Omega f = 0$ in an open, bounded set $\Omega \subset \mathbb{R}^d$ with $C^{2,\alpha}$-boundary for some $\alpha \in (0,1)$ and $d \leq 3$. Then $u \in C^2(\bar\Omega)$ and there exists a constant $C > 0$ such that

$$\|D^2 u\|_{C^0(\bar\Omega)} \leq C\|f\|_{C^1(\bar\Omega)} \tag{A.5}$$

with a constant $C = C(d,\alpha,\Omega)$.

Proof. Since Ω has a smooth $C^{2,\alpha}$-boundary and the right hand side of the Poisson equation is in $C^1(\bar{\Omega})$, the elliptic problem with constant coefficients admits an analogue result to the commonly treated Dirichlet case: u is in fact a $C^{2,\alpha}$-solution u with the estimate

$$\|D^2u\|_{C^{0,\alpha}(\bar{\Omega})} \leq C(\|u\|_{C^0(\bar{\Omega})} + \|f\|_{C^{0,\alpha}(\bar{\Omega})}).$$

To get an estimate on $\|u\|_{C^0(\bar{\Omega})}$ we split our solution u into its harmonic and potential part $u = v + w$, i.e.

$$\Delta v = 0 \qquad \Delta w = f \qquad \text{in } \Omega \tag{A.6}$$

$$\int_\Omega v = -\int_\Omega w \qquad \partial_\nu v = \partial_\nu w \qquad \text{on } \partial\Omega. \tag{A.7}$$

The contraints (A.7) result from (A.2). Using representations based on the fundamental solution $\mathcal{L}$ of the Laplacian

$$\mathcal{L}(x-y) := \mathcal{L}(|x-y|) = \begin{cases} c_d|x-y|^{2-d} & d > 2, \\ \frac{1}{2\pi}\log|x-y| & d = 2, \end{cases}$$

we have

$$w(x) = \mathcal{L} * f(x) = \int_\Omega \mathcal{L}(x-y)f(y)\,dy \tag{A.8}$$

$$v(x) = \int_{\partial\Omega} \mathcal{L}(x-y)\nabla w(y) \cdot \nu_\Omega\, do(y) + \bar{c} \tag{A.9}$$

where $\bar{c}$ originates from the integral contraint in (A.7). By the representations we see that v and w can be estimated uniformly in x by the $C^0(\Omega)$-norm of f. Thus we have the estimate (A.5) for $\|D^2u\|_{C^0(\Omega)}$. □

Theorem A.5. *Let Q be a quasilinear, uniformly elliptic differential operator in an open, bounded set $\Omega \subset \mathbb{R}^d$*

$$Qu = \sum_{i,j=1}^{d} a^{ij}(x, Du)D_{ij}u + b(x,u) \qquad \textit{for } u \in C^2(\Omega)$$

where $(a^{ij}(x,p))_{ij}$ is a symmetric and positive definite matrix, $(a^{ij}(x,p))_{ij}$ is continuously differentiable with respect to p for all $x \in \Omega$ and a^{ij}, b are continuous functions. Suppose that there exists a non-negative constant c_0 such that

$$\frac{b(x,z)sign(z)}{\sum_{i,j} a^{ij}(x,p)p_ip_j} \leq \frac{c_0}{|p|} \quad \forall\,(x,z,p) \in \Omega \times \mathbb{R} \times \mathbb{R}^d.$$

Then, for every $u \in C^0(\bar{\Omega}) \cap C^2(\Omega)$ satisfying $Qu \geq 0$ in Ω, we have

$$\sup_{x\in\Omega} \big[u(x)\,|u|(x)\big] \leq \sup_{x\in\partial\Omega} \big[u^+(x)\,|u|(x)\big].$$

Proof. See Theorem 10.3 in [GilTru98] with $\mu_2 = 0$ in notation there. Note that although that this theorem uses Theorem 10.1 from [GilTru98], it is not necessary that the coefficient functions have the properties of the assumptions from [GilTru98, Theorem 10.1]. Especially property (iii) therein which requires b to be non-increasing in z becomes redundant for Theorem 10.3. □

Theorem A.6. *Let X, Y be compact metrizable, separable metric spaces, μ a probability measure on X, let $\pi\colon X \to Y$ be a Borel map and let $\nu := \pi_\sharp \mu$ be the push-forward propability measure of μ onto Y. Then there exists a ν-almost everywhere uniquely determined Borel family of probability measures $\{\mu_y\}_{y\in Y}$ on X such that*

$$\mu_y(X \setminus \pi^{-1}(y)) = 0 \quad \text{for } \nu\text{-almost every } y \in Y \tag{A.10}$$

and

$$\int_X f(x)d\mu(x) = \int_Y \left(\int_{\pi^{-1}(y)} f(x)d\mu_y(x) \right) d\nu(y) \tag{A.11}$$

for every Borel map $f\colon X \to [0, \infty]$.

Proof. This is proven in [AmGiSa00] [Thm. 5.3.1] using the fact that every compact metrizable space is a Radon space, Proposition see A.7. □

Proposition A.7. *A compact metrizable space is a Radon space.*

Proof. See [Schw88] chapter I.II.3. □

Remark. A *Radon space* is defined as a Hausdorff space where every finite Borel measure is a Radon measure, see [Schw88].

A.2 Calculations for the rotation-symmetric case

The actual calculations of Subsection 4.2 are done using the program Mathematica which is able to solve equations symbolically. The reason for the usage is that we have five variables representing the deformation vector (see equations (4.38)-(4.40)). But we want to study the effect of the outer force S^* and the Lamé-constants (4.35), four of them are present: two for each phase. So, the five variables are solved depending on five parameters and plugged into equations (4.28) and (4.29). As we have seen, the sign of the difference $\hat{w}_2 - \hat{w}_0$ is crucial for the question whether the inner particle grows or shrinks.

We assume that $\nu = 1/3$, as it is proposed in [Brae91] for most cases. This reduces the complexity of our problem by two parameters. We will see that this is still complex enough. Somehow the introduction of the quotient $E := E^+/E^-$ turned out to be useful.

The result which is presented here is the difference $\hat{w}_2 - \hat{w}_0$. This is a complicated quotient, so we start slowly with the denominator of it.

The denominator of $\hat{w}_2 - \hat{w}_0$ is

$$24E^+rR\big((d-1)(E-1)(d-1+(d+1)E)R^d(R^d-r^d)+ \\ ((d^2-1)(E-1)^2r^d-(1+d+(d-1)E)(-1+d+(d+1)E)R^d)\bar{R}^d\big)^2.$$

For admissible variables it is clearly non-negative.

The nominator of $\hat{w}_2 - \hat{w}_0$ is

$$d\Big(48(d-1)^2drR\left(r^d-R^d\right)^2\bar{R}^{2d}(S^*)^2+24(d^2-1)^2E^5E^-(r+R)\left(r^d-R^d\right)^2\left(R^d-\bar{R}^d\right)^2\sigma \\ +8(d-1)E\left(r^d-R^d\right)\big(-4drR\left((5d-4)r^d+(3d+4)R^d\right)\bar{R}^{2d}(S^*)^2+ \\ 3(d-1)E^-\left(r^d-R^d\right)\left((1+d)(q^+-q^-)rR\bar{R}^d\left(-(d-1)R^d+(2d-1)\bar{R}^d\right)S^*+ \\ (r+R)\left((d-1)R^d+(1+d)\bar{R}^d\right)^2\sigma\right)\big)-\left(d^2-1\right)E^4\left(r^d-R^d\right) \\ \Big(-9(1+d)^2{E^-}^2(q^+-q^-)^2rR\left(r^d-R^d\right)\bar{R}^d\left(2(d-1)R^d-(d-2)\bar{R}^d\right) \\ -16drR\left(r^d-R^d\right)\bar{R}^{2d}(S^*)^2+24E^-\left((1+d)(q^+-q^-)rR\left(r^d-R^d\right)\bar{R}^d\left((d-1)R^d+\bar{R}^d\right)S^*-\right. \\ \left.4(r+R)\left(R^d-\bar{R}^d\right)\left((d-1)R^d\left(R^d-r^d\right)+\left(\left(d^2-1\right)r^d+\left(1+d^2\right)R^d\right)\bar{R}^d\right)\sigma\right)\Big)+ \\ (d-1)E^2\left(r^d-R^d\right) \\ \Big(9(d-1)(1+d)^2{E^-}^2(q^+-q^-)^2rR\left(r^d-R^d\right)\bar{R}^d\left(-2(d-1)R^d+(d-2)\bar{R}^d\right)+ \\ 32drR\left((6d-3)r^d+(3+10d)R^d\right)\bar{R}^{2d}(S^*)^2+24E^- \\ \left((1+d)(q^+-q^-)rR\bar{R}^d\left((d-3)(d-1)R^d\left(r^d-R^d\right)-\right.\right. \\ \left.\left((3+d(4d-5))r^d+(1+d)(8d-3)R^d\right)\bar{R}^d\right)S^* \\ -4(r+R)\left((d-1)R^d+(1+d)\bar{R}^d\right)\left((d-1)R^d\left(R^d-r^d\right)+\right. \\ \left.\left.\left(\left(d^2-1\right)r^d+\left(1+d^2\right)R^d\right)\bar{R}^d\right)\sigma\right)\Big)- \\ 2E^3\Big(9(d-1)(1+d)^2{E^-}^2(q^+-q^-)^2rR\left(r^d-R^d\right)\bar{R}^d \\ \left(-2(d-1)R^d\left(R^d-r^d\right)+\left(-(d-2)r^d+\left(d-2+4d^2\right)R^d\right)\bar{R}^d\right)+ \\ 16(d-1)d^2rR\left(r^d-R^d\right)\left(3r^d+5R^d\right)\bar{R}^{2d}(S^*)^2+ \\ 12E^-\left(-\left(d^2-1\right)(q^+-q^-)rR\left(r^d-R^d\right)\bar{R}^d\right. \\ \left((d-1)(3+d)R^d\left(r^d-R^d\right)+\left((3+d(2d-1))r^d+\left(d-3+10d^2\right)R^d\right)\bar{R}^d\right)S^*+ \\ 2(r+R)\Big(\left(d-1\right)^2\left(d^2-3\right)R^{2d}\left(r^d-R^d\right)^2+2(d-1)R^d\left(r^d-R^d\right)\Big(3\left(d^2-1\right)r^d+ \\ \left(3+d^2\right)R^d\Big)\bar{R}^d-\Big(3\left(d^2-1\right)^2r^{2d}+2\left(d^4+2d^2-3\right)r^dR^d+\left(3+2d^2+3d^4\right)R^{2d}\Big)\bar{R}^{2d}\Big)\sigma\Big)\Big)\Big).$$

Note that this is a polynomial in the various parameters. In Subsection 4.2.2 different cases are studied.

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