

## MULTI-COMPONENT ALLEN-CAHN EQUATION FOR ELASTICALLY STRESSED SOLIDS

THOMAS BLESSEN, ULRICH WEIKARD

ABSTRACT. The vector-valued Allen-Cahn equations are combined with elasticity where a linear stress-strain relationship is assumed. A short physical derivation of the generalised model is given and global existence and uniqueness of the solution are shown under suitable growth conditions on the non-linearity.

### 1. INTRODUCTION

The Allen-Cahn equation, introduced in [2], provides a well-established framework for the mathematical description to free boundary problems for phase transitions. Unlike sharp interface models, it postulates a diffuse interface with a small thickness  $\gamma > 0$ . The equations have been the subject of intense mathematical investigations, see for instance [27, 5, 1, 9, 14, 15]; and adequate numerical methods have been developed for their solution, see [25, 23], that contain also references to other numerical work.

The Allen-Cahn equation has been generalised in many directions, see [10, 24] for a generalisation to the phase field equations; [21], where also the vector-valued system of Allen-Cahn equations is derived; [6], where a statistical framework is considered, and finally [27] for a mixed Allen-Cahn/Cahn-Hilliard formulation.

The physical applications of the Allen-Cahn system are numerous. An overview over the Allen-Cahn and phase field equations is [11], in [20] an overview over the Cahn-Hilliard equation with elasticity is found. Furthermore we mention [26] and [22] with applications to dislocations and lattice instabilities, [3], where droplet motion is described, [5] for the study of travelling waves, [28] for applications to crystallisation, and [7] for diffusion induced segregation phenomena.

In this article we consider a generalisation of the vector-valued system of Allen-Cahn equations to linear elasticity. To this end we will first give a short physical derivation of the complete model, then show existence and uniqueness of a solution to the generalised system.

The existence proof can be roughly split into two parts. Part I, presented in sections 2 to 4, treats the case of polynomial free energy densities that fulfill the mild growth conditions stated in Section 2.3. The second part, starting in Section 6,

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treats the physically relevant case of logarithmic free energy densities and makes use of the results shown in Part I. The employed mathematical methods consist in starting from the time-discrete formulation and finding suitable uniform estimates independent of the time step  $\tau > 0$  which by well-known compactness results allow to pass to the limit  $\tau \rightarrow 0$ . A former version of this argument can be found in [4] and is classical by now. Our approach will follow closely [17, 18, 19] where the elastic Cahn-Hilliard model is treated.

**1.1. Derivation of the Model.** Let  $\Omega \subset \mathbb{R}^D$ ,  $1 \leq D \leq 3$  be a bounded domain with Lipschitz boundary. We introduce the vector  $u := (u_1, \dots, u_n)$  of non-conserved order parameters. Depending on the physical context,  $u_i$  can be either the concentration, or the density, or the volume fraction of the  $i$ -th phase.

These quantities fulfill for  $1 \leq i \leq n$

$$u_i \geq 0, \quad u_i \in H^{1,2}(\Omega), \quad \sum_{i=1}^n u_i = 1.$$

By  $H^{m,2}(\Omega)$  we denote the Sobolev space of  $m$ -times weakly differentiable functions in the Hilbert space  $L^2(\Omega)$ , by  $H_0^{m,2}(\Omega)$  the closure of  $C_0^\infty(\Omega)$  w.r.t.  $\|\cdot\|_{H^{1,2}(\Omega)}$ . By  $\|\cdot\|_{H^1}$  we always mean  $\|\cdot\|_{H^{1,2}(\Omega)}$ .  $C_0^\infty(\Omega) := \bigcap_{m=0}^\infty C_0^m(\Omega)$  where  $C_0^m(\Omega)$  is the space of  $m$ -times continuously differentiable functions over  $\Omega$  with compact support.

In order to describe elastic effects we consider the displacement field  $v(x)$  which describes the position of a material point  $x$  in the undeformed body after deformation. We assume that the displacement gradient is small, such that the strain tensor can be approximated by

$$\mathcal{E} = \mathcal{E}(v) = \mathcal{E}_{ij}(v) := \frac{1}{2}(\partial_i v_j + \partial_j v_i).$$

We postulate that the system free energy is of the generalised Landau-Ginzburg form

$$F(u(t), \mathcal{E}(v(t))) = F^{\text{out}}(\mathcal{E}(v(t))) + \int_{\Omega} \left( \frac{\gamma^2}{2} \sum_{i=1}^n |\nabla u_i(x, t)|^2 + f(u(x, t), \mathcal{E}(v(x, t))) \right) dx. \quad (1.1)$$

In this formulation, the first term represents energy effects due to applied outer forces,

$$F^{\text{out}}(\mathcal{E}(v)) := \int_{\Omega} \overline{W}(\mathcal{E}(v)).$$

We assume that there are no external body forces and that the tractions applied to  $\partial\Omega$  are dead loads and equal  $\overline{S}\vec{n}$ , where  $\vec{n}$  is the unit outer normal to  $\partial\Omega$ . We assume that the symmetric tensor  $\overline{S}$  defined by this property is constant, i.e. independent of time  $t$ . The work necessary to transform the undeformed body into the state with corresponding displacement vector  $v(t)$  is therefore

$$- \int_{\partial\Omega} v \cdot \overline{S}\vec{n} = - \int_{\Omega} \nabla v : \overline{S} = - \int_{\Omega} \mathcal{E}(v) : \overline{S}$$

and we find that  $\overline{W}(\mathcal{E}(v)) := -\mathcal{E}(v) : \overline{S}$  describes the energy density of the applied outer forces.

The term  $\frac{\gamma^2}{2} \sum_{i=1}^n |\nabla u_i|^2$  in (1.1) represents the interfacial energy of the transition layers. Here we assume for simplicity that the contributions enter with the same weight for every interface between any two phases.

The last term  $f(u, \mathcal{E}(v))$  in (1.1) represents the free energy density. The computations in this article are based on the equality

$$f(u, \mathcal{E}(v)) = \bar{f}(u) + W^{\text{el}}(u, \mathcal{E}(v))$$

with suitable structure and growth conditions on  $\bar{f}$ , see Section 2.3.  $W^{\text{el}}$  is the contribution of the elastic energy to  $f$ . It was first studied by Eshelby, [16]. By Hooke's law, a possible ansatz for  $W^{\text{el}}$  is

$$W^{\text{el}}(u, \mathcal{E}) := \frac{1}{2} (\mathcal{E} - \bar{\varepsilon}(u)) : C(u) (\mathcal{E} - \bar{\varepsilon}(u)). \quad (1.2)$$

We assume the linear relationship (*Vegard's law*)

$$\bar{\varepsilon}(u) := \sum_{i=1}^n u_i \bar{\varepsilon}_i, \quad (1.3)$$

where  $\bar{\varepsilon}_i := \bar{\varepsilon}(e_i)$  and  $e_i$  is the  $i$ -th basis vector of  $\mathbb{R}^n$ . This means  $\bar{\varepsilon}(e_i)$  is the eigenstrain when the system is equal to the  $i$ th pure component.  $C(u)$  is the elasticity tensor that maps symmetric tensors in  $\mathbb{R}^{D \times D}$  onto itself. We assume that  $C$  is symmetric and positive definite. Instead of (1.2) other forms of  $W^{\text{el}}$  are permitted as long as Assumption (A4) in Section 2.3 remains valid.

We define the time evolution of the unconserved order parameter  $u$  as gradient flow of the free energy,

$$\int_{\Omega} \partial_t u = - \frac{\delta}{\delta u} F(u(t), \mathcal{E}(v(t))).$$

Thus for large time  $t$ ,  $u(t)$  tends to a local minimiser of  $F$ .

The mechanical equilibrium is attained on a much faster time scale than the time scale significant for diffusion. Therefore we will assume a quasi-static elastic equilibrium, i.e. the displacement  $v$  is obtained by solving the elliptic equation

$$\operatorname{div}(S) = 0 \quad \text{in } \Omega$$

with the stress tensor

$$S := \partial_{\varepsilon} W^{\text{el}}(u, \mathcal{E}(v)).$$

Hence, for a given stop time  $T > 0$  we end up with the following model:

*Find for  $t \geq 0$  a solution pair  $(u, v)$  such that in  $\Omega_T := \Omega \times (0, T)$*

$$\partial_t u = \gamma^2 \Delta u - P(\partial_u f(u, \mathcal{E}(v))), \quad (1.4)$$

$$\operatorname{div}(S) = 0, \quad (1.5)$$

$$S = \partial_{\varepsilon} W^{\text{el}}(u, \mathcal{E}(v)), \quad (1.6)$$

with the initial data for  $t = 0$  in  $\Omega$

$$u(\cdot, 0) = u_0(\cdot) \quad (1.7)$$

and the boundary conditions for  $t > 0$  in  $\partial\Omega$

$$u = u_d, \quad S \cdot \vec{n} = \bar{S} \cdot \vec{n}. \quad (1.8)$$

The projection operator  $P$  in (1.4) is due to algebraic constraints on  $\partial_u f(u, \mathcal{E}(v))$ . This is explained in the subsequent section.

The boundary condition  $S \cdot \vec{n} = \bar{S} \cdot \vec{n}$  on  $\partial\Omega$  determines  $v$  only up to infinitesimal rigid displacements (these are translations and infinitesimal rotations). This fact is well-known for formulations that depend on a linearised strain tensor  $\mathcal{E}$ . The resulting non-uniqueness in  $v$  is of no importance as  $v$  only enters through the symmetric term  $\mathcal{E}(v)$ .

## 2. PRELIMINARIES TO EXISTENCE THEORY

In this section we discuss the existence theory to the sharp interface model (1.4)-(1.8). We will show that under suitable growth conditions on the free energy density, stated for polynomial  $f$  in Section 2.3 and for logarithmic energies in Section 6, discrete solutions to the implicit time discretisation exist. A-priori estimates allow to pass to the limit showing the existence of solutions to the model first with polynomial free energy. This result is then used to generalise to logarithmic free energies.

We will carry out the proof for classical Dirichlet boundary data, i.e. set w.l.o.g.  $u_d = 0$  in (1.8). Other boundary conditions are shortly discussed in the remark at the end of this section. We begin by collecting general properties of the model and necessary tools that will be needed in the sequel.

The vector of order parameters lies inside the simplex  $\Sigma$ ,

$$u \in \Sigma := \left\{ u' = (u'_1, \dots, u'_n) \in \mathbb{R}^n : \sum_{i=1}^n u'_i = 1 \right\}. \quad (2.1)$$

Notice that the condition  $0 \leq u_i \leq 1$  in  $\Omega$  may be violated for polynomial free energies considered in the first part of this section.

If we write (1.4) as  $\partial_t u = w$ , as a consequence of (2.1),  $w$  fulfills  $\sum_{i=1}^n w_i = 0$ . Thus, with  $e := (1, \dots, 1) \in \mathbb{R}^n$ , the right hand side  $w$  satisfies  $w = P(z)$  for some  $z \in \mathbb{R}^n$ , where

$$P(z) := z - \frac{1}{n}(z \cdot e)e$$

is the projection of  $\mathbb{R}^n$  to

$$T\Sigma := \left\{ u' = (u'_1, \dots, u'_n) \in \mathbb{R}^n : \sum_{i=1}^n u'_i = 0 \right\},$$

the tangent space to  $\Sigma$ . Let

$$\begin{aligned} X_1 &:= \{ u' \in H_0^1(\Omega; \mathbb{R}^n) : u' \in \Sigma \text{ almost everywhere in } \Omega \}, \\ X_2 &:= \{ v' \in H^1(\Omega, \mathbb{R}^D) : (v', w)_{H^1} = 0 \text{ for all } w \in X_{\text{ird}} \}, \end{aligned}$$

where

$$X_{\text{ird}} = \{ v \in H^1(\Omega, \mathbb{R}^D) : \text{there exist } b \in \mathbb{R}^D, A \in \mathbb{R}^{D \times D} \text{ such that } v(x) = Ax + b \}$$

is the space of all infinitesimal rigid displacements.

Since we have (classical) Dirichlet boundary conditions for the equations of conservation of mass, we consider the space of test functions

$$Y := H_0^{1,2}(\Omega; \mathbb{R}^n)$$

and its dual

$$(H_0^{1,2}(\Omega; \mathbb{R}^n))' = H^{-1,2}(\Omega; \mathbb{R}^n).$$

**Remark:** If we replace the Dirichlet conditions for  $u$  by a Neumann boundary condition or periodic boundary conditions, a (generalised) Poincaré inequality holds in  $H^{1,2}(\Omega)$  and all the results found below continue to hold.

**2.1. The weak formulation.** A pair  $(u, v) \in L^2(0, T; H_0^{1,2}(\Omega; \mathbb{R}^n)) \times L^2(0, T; X_2)$  is called a *weak solution of (1.4)-(1.8)* if

$$-\int_{\Omega_T} \partial_t \xi \cdot (u - u_0) + \gamma^2 \int_{\Omega_T} \nabla u : \nabla \xi + \int_{\Omega_T} P(\partial_u f(u, \mathcal{E}(v))) \cdot \xi = 0 \quad (2.2)$$

for all  $\xi \in L^2(0, T; H_0^1(\Omega; \mathbb{R}^n)) \cap L^\infty(\Omega_T; \mathbb{R}^n)$  with  $\partial_t \xi \in L^2(\Omega_T)$ ,  $\xi(T) = 0$ , and

$$\int_{\Omega_T} W^{\text{el}}(u, \mathcal{E}(v)) : \nabla \zeta = \int_{\Omega_T} \bar{S} : \nabla \zeta. \quad (2.3)$$

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

**2.2. The implicit time discretisation.** We fix an  $M \in \mathbb{N}$  and set  $h := \frac{T}{M}$ . For  $m \geq 1$  and given  $u^{m-1} \in X_1$  consider

$$\frac{u^m - u^{m-1}}{h} = \gamma^2 \Delta u - P(\partial_u f(u^m, \mathcal{E}(v^m))), \quad (2.4)$$

$$\text{div}(S^m) = 0, \quad (2.5)$$

$$S^m = \partial_\varepsilon W^{\text{el}}(u^m, \mathcal{E}(v^m)). \quad (2.6)$$

**2.3. Structural Assumptions.** To establish the existence of weak solutions in the sense of Section 2.1, the following assumptions are made:

(A1)  $\Omega \subset \mathbb{R}^D$  is a bounded domain with Lipschitz boundary.

(A2) The free energy density  $f$  can be written as

$$f(u', \mathcal{E}(v')) = f^1(u') + f^2(u') + W^{\text{el}}(u', \mathcal{E}(v')) \quad \text{for all } u' \in \mathbb{R}^n, v' \in \mathbb{R}^D$$

with  $f^1 \in C^1(\mathbb{R}^n; \mathbb{R})$  and convex. Additionally we postulate

(A2.1)  $f^1 \geq 0$ .

(A2.2) For all  $\delta > 0$  there exists a constant  $C_\delta > 0$  such that

$$|\partial_u f^1(u')| \leq \delta f^1(u') + C_\delta \quad \text{for all } u' \in \Sigma.$$

(A2.3) There exists a constant  $C_1 > 0$  such that

$$|\partial_u f^2(u')| \leq C_1(|u'| + 1) \quad \text{for all } u' \in \Sigma.$$

(A3) The initial datum  $u_0$  fulfills  $f(u_0, \mathcal{E}(v_0)) < \infty$ , where  $v_0$  is the solution of (2.3).

(A4) The elastic energy density  $W^{\text{el}} \in C^1(\mathbb{R}^n \times \mathbb{R}^{D \times D}; \mathbb{R})$  satisfies

(A4.1)  $W^{\text{el}}(u', \mathcal{E}')$  only depends on the symmetric part of  $\mathcal{E}' \in \mathbb{R}^{D \times D}$ , i.e.

$$W^{\text{el}}(u', \mathcal{E}') = W^{\text{el}}(u', (\mathcal{E}')^t) \quad \text{for all } u' \in \mathbb{R}^n \text{ and } \mathcal{E}' \in \mathbb{R}^{D \times D}.$$

(A4.2)  $\partial_\varepsilon W^{\text{el}}(u', \cdot)$  is strongly monotone uniformly in  $u'$ , i.e. there exists a  $c_1 > 0$  such that for all symmetric  $\mathcal{E}'_1, \mathcal{E}'_2 \in \mathbb{R}^{D \times D}$ ,

$$(\partial_\varepsilon W^{\text{el}}(u', \mathcal{E}'_2) - \partial_\varepsilon W^{\text{el}}(u', \mathcal{E}'_1)) : (\mathcal{E}'_2 - \mathcal{E}'_1) \geq c_1 |\mathcal{E}'_2 - \mathcal{E}'_1|^2.$$

(A4.3) There exists a constant  $C_1 > 0$  such that for all  $u' \in \Sigma$  and all symmetric  $\mathcal{E}' \in \mathbb{R}^{D \times D}$ ,

$$\begin{aligned} |W^{\text{el}}(u', \mathcal{E}')| &\leq C_1(|\mathcal{E}'|^2 + |u'|^2 + 1), \\ |\partial_u W^{\text{el}}(u', \mathcal{E}')| &\leq C_1(|\mathcal{E}'|^2 + |u'|^2 + 1), \\ |\partial_\varepsilon W^{\text{el}}(u', \mathcal{E}')| &\leq C_1(|\mathcal{E}'| + |u'| + 1). \end{aligned}$$

(A5) The energy density of the applied outer forces is given by  $\overline{W}(\mathcal{E}') = -\mathcal{E}' : \overline{S}$  where  $\overline{S}$  is a symmetric constant tensor.

For the rest of this article, we assume without further stating that the assumptions (A1)-(A5) hold.

### 3. EXISTENCE OF SOLUTIONS TO THE TIME DISCRETE SCHEME

For each time step  $m \geq 1$  in the implicit time discretisation (2.4)-(2.6), given time step size  $h > 0$ , and given  $u^{m-1} \in X_1$  we define the discrete energy functional

$$F^{m,h}(u', v') := F(u', \mathcal{E}(v')) + \frac{1}{2h} \|u' - u^{m-1}\|_{L^2}^2.$$

**Lemma 3.1** (Existence of a minimiser). *For given  $u^{m-1} \in X_1$  and any  $h > 0$  the functional  $F^{m,h}$  possesses a minimiser  $(u^m, v^m)$  in  $X_1 \times X_2$ .*

*Proof.* The proof is an application of the direct method in the calculus of variations. Combined, (A4.2), (A4.3) imply that  $W^{\text{el}}(u', \mathcal{E}') \geq C(|\mathcal{E}'|^2 - |u'|^2) - C$  for a constant  $C > 0$ . With Korn's inequality, see for instance [12], this guarantees the coercivity of  $F$  with respect to  $v \in X_2$ . Similarly, the term  $\gamma^2 \int_\Omega \sum_{i=1}^n |\nabla u_i|^2$  in the definition of  $F$  guarantees with the Poincaré inequality the coercivity of  $F$  w.r.t.  $u \in X_1$ . Using (A2) on  $f^1$  and  $f^2$  we thus find that the functional  $F^{m,h}$  is weakly lower semicontinuous and coercive in  $X_1 \times X_2$  and hence possesses a minimiser.  $\square$

The following lemma shows that the energy functional  $F^{m,h}$  is the correct one and corresponds to the implicit time discretisation (2.4)-(2.6).

**Lemma 3.2** (Euler-Lagrange equations). *The minimiser  $(u^m, v^m) \in X_1 \times X_2$  of  $F^{m,h}$  fulfills*

$$\int_\Omega \frac{u^m - u^{m-1}}{h} \cdot \xi + \int_\Omega \gamma^2 \nabla u^m : \nabla \xi + \int_\Omega P(\partial_u f(u^m, \mathcal{E}(v^m))) \cdot \xi = 0 \quad (3.1)$$

for all  $\xi \in Y \cap L^\infty(\Omega; \mathbb{R}^n)$ ,

$$\int_\Omega \partial_\varepsilon W^{\text{el}}(u^m, \mathcal{E}(v^m)) : \nabla \zeta = \int_\Omega \overline{S} : \nabla \zeta \quad \text{for all } \zeta \in H^1(\Omega; \mathbb{R}^D). \quad (3.2)$$

*Proof.* We choose directions  $\xi \in Y \cap L^\infty(\Omega; \mathbb{R}^n)$  with  $\sum_{i=1}^n \xi_i = 0$ ,  $\zeta \in X_2 \cap L^\infty(\Omega; \mathbb{R}^D)$  and determine variations of  $F^{m,h}(u, v)$  with respect to  $u$  and  $v$  for  $\xi, \zeta$ . The variation w.r.t.  $u$  is

$$\lim_{s \rightarrow 0} \left( (F^{m,h}(u^m + s\xi, v^m) - F^{m,h}(u^m, v^m))s^{-1} \right). \quad (3.3)$$

Since  $f^1$  is convex, we have

$$f^1(u^m) \geq f^1(u^m + s\xi) - s \partial_u f^1(u^m + s\xi) \cdot \xi.$$

This implies

$$\begin{aligned} f^1(u^m + s\xi) &\leq f^1(u^m) + |s\partial_u f^1(u^m + s\xi)| \|\xi\|_{L^\infty} \\ &\leq f^1(u^m) + |s| f^1(u^m + s\xi) \|\xi\|_{L^\infty} + C|s|. \end{aligned}$$

The last is by Assumption (A2.2) with  $\delta = 1$ . Hence, for  $s$  small enough, we find

$$\left| \frac{f^1(u^m + s\xi) - f^1(u^m)}{s} \right| \leq C(f^1(u^m) + 1).$$

Lebesgue’s dominated convergence theorem and Assumption (A2.3) imply

$$\lim_{s \rightarrow 0} \frac{1}{s} \left( \int_{\Omega} (f^1 + f^2)(u^m + s\xi) - (f^1 + f^2)(u^m) \right) = \int_{\Omega} (\partial_u f^1 + \partial_u f^2)(u^m) \cdot \xi.$$

With the help of (A4.3) we find

$$\begin{aligned} &\lim_{s \rightarrow 0} \int_{\Omega} s^{-1} \left( W^{\text{el}}(u^m + s\xi, \mathcal{E}(v^m + s\zeta)) - W^{\text{el}}(u^m, \mathcal{E}(v^m)) \right) \\ &= \int_{\Omega} \left( \partial_u W^{\text{el}}(u^m, \mathcal{E}(v^m))\xi + \partial_\varepsilon W^{\text{el}}(u^m, \mathcal{E}(v^m)) : \nabla \zeta \right). \end{aligned}$$

The variation of the quadratic form  $u \mapsto \frac{1}{2h} \|u^m - u^{m-1}\|_{L^2}^2$  yields

$$\lim_{s \rightarrow 0} \left( s^{-1}(2h)^{-1} (\|u^m + s\xi - u^{m-1}\|_{L^2}^2 - \|u^m - u^{m-1}\|_{L^2}^2) \right) = \left( \frac{u^m - u^{m-1}}{h}, \xi \right)_{L^2}.$$

Taking into account that  $u^m - u^{m-1}$  as well as  $\nabla u^m : \nabla \xi$  for every  $\xi$  lie on  $T\Sigma$ , this finally yields (3.1). To derive (3.2) we vary  $F^{m,h}$  with respect to  $v$ . From the symmetry of  $\partial_\varepsilon W^{\text{el}}$  and  $\bar{S}$  we find (3.2).  $\square$

**3.1. Uniform estimates.** In the preceding section we proved the existence of a discrete solution  $(u^m, v^m)$  for  $1 \leq m \leq M$  and arbitrary  $M \in \mathbb{N}$ . We define the piecewise constant extension  $(u_M, v_M)$  of  $(u^m, v^m)_{1 \leq m \leq M}$  by

$$(u_M(t), v_M(t)) := (u_M^m, v_M^m) := (u^m, v^m) \quad \text{for } t \in ((m-1)h, mh]$$

with  $u_M(0) = u_0$ , and  $v_M(0)$  given by Equation (2.6).

The piecewise linear extension  $(\bar{u}_M, \bar{v}_M)$  for  $t = (\beta m + (1 - \beta)(m - 1))h$  with appropriate  $\beta \in [0, 1]$  is given by the interpolation

$$(\bar{u}_M, \bar{v}_M)(t) := \beta(u_M^m, v_M^m) + (1 - \beta)(u_M^{m-1}, v_M^{m-1}).$$

**Lemma 3.3** (A-priori estimates). *The following a-priori estimates are valid.*

(a) *For all  $M \in \mathbb{N}$  and all  $t \in [0, T]$  we have the dissipation inequality*

$$F(u_M, \mathcal{E}(v_M))(t) + \frac{1}{2} \int_{\Omega_t} |\partial_t \bar{u}_M|^2 \leq F(u_0, \mathcal{E}(v_0)).$$

(b) *There exists a constant  $C > 0$  such that*

$$\sup_{0 \leq t \leq T} \left\{ \|u_M(t)\|_{H^1} + \|v_M(t)\|_{H^1} \right\} \leq C, \tag{3.4}$$

$$\sup_{0 \leq t \leq T} \int_{\Omega} f^1(u_M(t)) + \|\partial_t \bar{u}_M\|_{L^2(\Omega_T)} \leq C. \tag{3.5}$$

*Proof.* Since  $(u^m, v^m)$  is a minimiser of  $F^{m,h}$ , it holds for every  $m \geq 1$

$$F(u^m, \mathcal{E}(v^m)) + \frac{1}{2h} \|u^m - u^{m-1}\|_{L^2}^2 \leq F(u^{m-1}, \mathcal{E}(v^{m-1})). \quad (3.6)$$

After writing  $u^m - u^{m-1}$  as a time derivative, iterating (3.6) yields

$$F(u_M^m, \mathcal{E}(v_M^m)) + \frac{1}{2} \int_0^{mh} \|\partial_t \bar{u}_M\|_{L^2}^2 d\tau \leq F(u_0, \mathcal{E}(v_0)).$$

Using the assumptions (A2)-(A4) and with the help of the inequalities of Poincaré and Korn, this proves the lemma.  $\square$

For the linear interpolation  $\bar{u}_M$  of  $u_M^m$ , the Euler-Lagrange equation (3.1) can be rewritten as

$$\int_{\Omega} \partial_t \bar{u}_M(t) \cdot \xi + \int_{\Omega} \gamma^2 \nabla u_M(t) : \nabla \xi + \int_{\Omega} P(\partial_u f(u_M(t), \mathcal{E}(v_M(t)))) \cdot \xi = 0 \quad (3.7)$$

for all  $\xi \in Y \cap L^\infty(\Omega; \mathbb{R}^n)$ , which holds for almost all  $t \in (0, T)$ . Equation (3.7) controls the variation of  $\bar{u}_M$  in time and, together with the uniform estimates of Lemma 3.3, allows to show compactness in time.

The following theorem is the first main result as it can also be used to proof convergence of numerical solution schemes. In the next part we will show that this limit is in fact a solution to (1.4)-(1.8).

**Theorem 3.4** (Compactness of  $(u_M, v_M)$ ). *There exists a constant  $C > 0$  such that for all  $t_1, t_2 \in [0, T]$*

$$\|\bar{u}_M(t_2) - \bar{u}_M(t_1)\|_{L^2} \leq C|t_2 - t_1|^{1/4}.$$

Furthermore, there are subsequences  $(u_M)_{M \in \mathcal{N}}$  and  $(v_M)_{M \in \mathcal{N}}$  with  $\mathcal{N} \subset \mathbb{N}$  and there are  $u \in L^\infty(0, T; H_0^1(\Omega))$  and  $v \in L^\infty(0, T; H^1(\Omega))$  such that

- (i)  $\bar{u}_M \rightarrow u$  in  $C^{0,\alpha}([0, T]; L^2(\Omega; \mathbb{R}^n))$  for all  $\alpha \in (0, \frac{1}{4})$ ,
- (ii)  $u_M \rightarrow u$  in  $L^\infty(0, T; L^2(\Omega; \mathbb{R}^n))$ ,
- (iii)  $u_M \rightarrow u$  almost everywhere in  $\Omega_T$ ,
- (iv)  $u_M \xrightarrow{*} u$  in  $L^\infty(0, T; H_0^1(\Omega; \mathbb{R}^n))$ ,
- (v)  $v_M \rightarrow v$  in  $L^2(0, T; H^1(\Omega))$ ,
- (vi)  $\partial_u f^k(u_M) \rightarrow \partial_u f^k(u)$  in  $L^1(\Omega_T)$  for  $k = 1, 2$

as  $M \in \mathcal{N}$  tends to infinity.

*Proof.* For chosen constant  $L > 0$  let

$$P_L(u') := \begin{cases} u' & \text{if } |u'| \leq L, \\ \frac{u'}{|u'|} L & \text{if } |u'| > L. \end{cases} \quad (3.8)$$

In (3.7) we test with  $\xi := P_L(\bar{u}_M(t_2) - \bar{u}_M(t_1))$ , where  $t_1, t_2 \in [0, T]$  with  $t_1 < t_2$ . After integration in time from  $t_1$  to  $t_2$  we obtain

$$\begin{aligned} & \|\bar{u}_M(t_2) - \bar{u}_M(t_1)\|_{L^2}^2 + \int_{t_1}^{t_2} \int_{\Omega} \gamma^2 \nabla u_M(t) : \nabla (\bar{u}_M(t_2) - \bar{u}_M(t_1)) dt \\ & + \int_{t_1}^{t_2} \int_{\Omega} P(\partial_u f(u_M(t), \mathcal{E}(v_M(t)))) P_L(\bar{u}_M(t_2) - \bar{u}_M(t_1)) dt = 0. \end{aligned}$$

The  $u_M^n$  are uniformly bounded in  $H^1(\Omega; \mathbb{R}^n)$ , therefore the linear interpolants  $u_M$  are uniformly bounded in  $L^\infty(0, T; H^1(\Omega; \mathbb{R}^n))$ . Thus we obtain

$$\begin{aligned} & \|\bar{u}_M(t_2) - \bar{u}_M(t_1)\|_{L^2}^2 \\ & \leq C \|\bar{u}_M\|_{L^\infty(H^1)} \int_{t_1}^{t_2} \left( \gamma^2 \|\nabla u_M(t)\|_{L^2} + \|(\partial_u f^1 + \partial_u f^2)(u_M(t))\|_{L^2} \right) dt \\ & \quad + C \|P_L \bar{u}_M\|_{L^\infty(\Omega_T)} \int_{t_1}^{t_2} \|\partial_u W^{\text{el}}(u_M(t), v_M(t))\|_{L^1} dt \\ & \leq C \|\bar{u}_M\|_{L^\infty(H^1)} (t_2 - t_1)^{1/2} \left( \|\nabla u\|_{L^2(\Omega_T)} + \|(\partial_u f^1 + \partial_u f^2)(u)\|_{L^2(\Omega_T)} \right) \\ & \quad + C \|P_L \bar{u}_M\|_{L^\infty(\Omega_T)} (t_2 - t_1) \|\partial_u W^{\text{el}}(u, v)\|_{L^\infty(L^1)}. \end{aligned}$$

Employing the a-priori estimate (3.4) and with the help of (A2.2), (A2.3) and (A4.3) we have proved

$$\|u_M(t_2) - u_M(t_1)\|_{L^2} \leq C |t_2 - t_1|^{1/4} \quad \text{for all } t_1, t_2 \in [0, T]$$

for a positive constant  $C$ . This is the equicontinuity of  $(u_M)_{M \in \mathbb{N}}$ .

The boundedness of  $(u_M)$  in  $L^\infty(0, T; H^1(\Omega))$  together with the fact that  $H^1$  is compactly embedded in  $L^2$  yields with the Arzelà-Ascoli theorem statement (i).

The claims (ii), (iii) and (iv) are shown as follows. Choose for  $t \in [0, T]$  values  $m \in \{1, \dots, M\}$  and  $\beta \in [0, 1]$  such that  $t = (\beta m + (1 - \beta)(m - 1))h$ . From the definition of  $\bar{u}$  we get at once

$$\begin{aligned} \|\bar{u}_M(t) - u_M(t)\|_{L^2} &= \|\beta u_M^m + (1 - \beta)u_M^{m-1} - u_M^m\|_{L^2} \\ &= (1 - \beta) \|u_M^m - u_M^{m-1}\|_{L^2} \leq Ch^{1/4}. \end{aligned}$$

This tends to zero as  $M$  becomes infinite. With the help of (i), this proves (ii). Since for a subsequence we have convergence almost everywhere, (iii) is proved, too. Claim (iv) is a direct consequence of Estimate (3.4) which gives the boundedness of  $u_M$  in  $L^\infty(0, T; H^1(\Omega; \mathbb{R}^n))$ .

The proof of (v) is contained in [17, Lemma 3.5].

To prove (vi), we first notice that by Assumption (A2),  $\partial_u f^1$  is a continuous function. Hence, by (iii),

$$\partial_u f^1(u_M) \rightarrow \partial_u f^1(u) \quad \text{almost everywhere in } \Omega_T.$$

The growth condition of Assumption (A2.2) on  $f^1$  now yields that for arbitrary  $\delta > 0$  and all measurable  $E \subset \Omega$

$$\int_E |\partial_u f^1(u_M)| \leq \delta \int_E f^1(u_M) + C_\delta |E| \leq \delta C + C_\delta |E|.$$

Therefore,  $\int_E |\partial_u f^1(u_M)| \rightarrow 0$  as  $|E| \rightarrow 0$  uniformly in  $M$  and by Vitali's theorem we find  $\partial_u f^1(u_M) \rightarrow \partial_u f^1(u)$  in  $L^1(\Omega_T)$  as  $M \in \mathbb{N}$  tends to infinity.

Assumption (A2.3) yields with Lebesgue's dominated convergence theorem accordingly

$$\partial_u f^2(u_M) \rightarrow \partial_u f^2(u).$$

□

## 4. GLOBAL EXISTENCE OF SOLUTIONS I

**Theorem 4.1** (Global existence of solutions for polynomial free energy). *Let the assumptions of Section 2.3 hold. Then there exists a weak solution  $(u, v)$  of (1.4)-(1.8) in the sense of Section 2.1 such that*

- (i)  $u \in C^{0, \frac{1}{4}}([0, T]; L^2(\Omega; \mathbb{R}^n))$ ,
- (ii)  $\partial_t u \in L^2(\Omega_T; \mathbb{R}^n)$ ,
- (iii)  $v \in L^2(0, T; H^1(\Omega))$ .

*Proof.* We are going to prove that  $(u, v)$  introduced in Theorem 3.4 is the desired weak solution in the sense of Section 2.1. From Equation (3.7) we learn

$$-\int_{\Omega_T} \partial_t \xi \cdot (\bar{u}_M - u_0) + \int_{\Omega_T} \gamma^2 \nabla u_M : \nabla \xi + \int_{\Omega_T} P(\partial_u f(u_M, \mathcal{E}(v_M))) \cdot \xi = 0$$

for all  $\xi \in L^2(0, T; Y)$  with  $\partial_t \xi \in L^2(\Omega_T)$  and  $\xi(T) = 0$ . In this equation we pass to the limit  $M \rightarrow \infty$  and exploit Theorem 3.4. The convergence of the linear expressions is clear. The convergence

$$\int_{\Omega_T} \partial_u f(u_M, \mathcal{E}(v_M)) \cdot \xi \rightarrow \int_{\Omega_T} \partial_u f(u, \mathcal{E}(v)) \cdot \xi$$

follows similar to the proof of Theorem 3.4 with Vitali's theorem by using the growth condition (A2.2) on  $f^1$ , (A2.3), Estimate (3.5), the almost everywhere convergence of  $u_M$  and the boundedness of  $\xi$ . The generalised Lebesgue convergence theorem, the growth condition (A4.3), and the strong convergence of  $\nabla v_M$  and  $u_M$  in  $L^2(\Omega)$  yield that we can pass to the limit in  $\int_{\Omega} \partial_u W^{\text{el}}(u_M, \mathcal{E}(v_M)) \cdot \xi$ . This implies (2.2).

Similarly we can pass to the limit in (3.2) and obtain (2.3). This is done in the same way as before by using once more growth condition (A4.3) and the strong convergence of  $\nabla v_M$  and  $u_M$  in  $L^2(\Omega)$ .  $\square$

## 5. UNIQUENESS OF THE SOLUTION

We show uniqueness of a solution to (1.4)-(1.6) under the simplifying assumption that

$$W^{\text{el}}(u', \mathcal{E}') = \frac{1}{2}(\mathcal{E}' - \bar{\varepsilon}(u')) : C(\mathcal{E}' - \bar{\varepsilon}(u')), \quad (5.1)$$

with a symmetric constant positive definite tensor  $C$  and with  $\bar{\varepsilon}(u')$  defined by (1.3).

The proof of the following theorem is straightforward and uses an integration in time method and a Gronwall argument.

**Theorem 5.1** (Uniqueness of solutions to the elastic Allen-Cahn system). *Let  $W^{\text{el}}$  be given by (5.1). Then the solution pair  $(u, v)$  obtained in Theorem 4.1 is unique in the spaces stated in this theorem.*

*Proof.* If there are two pairs of solutions  $(u^1, v^1)$ ,  $(u^2, v^2)$  to the equations (1.4)-(1.6), it holds for  $k = 1, 2$

$$\begin{aligned} \partial_t u^k &= \gamma^2 \Delta u^k - P(\partial_u f^1(u^k) + \partial_u f^2(u^k)) - P((\bar{\varepsilon}_i : C(\bar{\varepsilon}(v^k) - \bar{\varepsilon}(u^k)))_{1 \leq i \leq n}), \\ 0 &= \text{div}(C(\mathcal{E}(v^k) - \bar{\varepsilon}(u^k))). \end{aligned} \quad (5.2)$$

Let  $u := u^2 - u^1$  and  $v := v^2 - v^1$ . Then  $(u, v)$  solves the weak equation

$$\begin{aligned} \int_{\Omega_T} \partial_t u \cdot \xi &= - \int_{\Omega_T} \gamma^2 \nabla u : \nabla \xi - \int_{\Omega_T} (\partial_u(f^1 + f^2)(u^2) - \partial_u(f^1 + f^2)(u^1)) \cdot P\xi \\ &\quad - \int_{\Omega_T} (\bar{\varepsilon}_i : C(\mathcal{E}(v) - \bar{\varepsilon}(u)))_{1 \leq i \leq n} \cdot P\xi \end{aligned} \tag{5.3}$$

for every  $\xi \in L^2(0, T; Y) \cap L^\infty(\Omega_T; \mathbb{R}^n)$  with  $\partial_t \xi \in L^2(\Omega_T)$  and  $\xi(T) = 0$ . Let  $t_0 \in (0, T)$ . We choose  $P_L(u^2 - u^1)\mathcal{X}_{(0, t_0)}$  as a test function in the difference of the weak formulations of (5.2), where  $L > 0$  and  $P_L(u)$  is defined as in (3.8). In the limit  $L \rightarrow \infty$  the terms with  $P_L(u)$  are replaced by  $u$  and we find

$$\int_{\Omega_{t_0}} C(\mathcal{E}(v) - \bar{\varepsilon}(u)) : \mathcal{E}(v) = 0. \tag{5.4}$$

Similarly we choose  $\xi := P_L(u^2 - u^1)\mathcal{X}_{(0, t_0)}$  as test function in (5.3) and in the limit  $L \rightarrow \infty$  we obtain with the help of (5.4)

$$\begin{aligned} \frac{1}{2} \int_{\Omega_{t_0}} \frac{d}{dt} |u|^2 &= - \int_{\Omega_{t_0}} \gamma^2 \nabla u : \nabla u - \int_{\Omega_{t_0}} (\mathcal{E}(v) - \bar{\varepsilon}(u)) : C(\mathcal{E}(v) - \bar{\varepsilon}(u)) \\ &\quad - \int_{\Omega_{t_0}} (\partial_u(f^1 + f^2)(u^2) - \partial_u(f^1 + f^2)(u^1)) \cdot (u^2 - u^1). \end{aligned}$$

The convexity of  $f^1$  yields

$$\partial_u(f^1(u^2) - f^1(u^1)) \cdot (u^2 - u^1) \geq 0$$

and due to  $u(t = 0) = 0$  we end up with

$$\frac{1}{2} \int_{\Omega_{t_0}} \frac{d}{dt} |u|^2 = \frac{1}{2} \|u(t_0)\|_{L^2}^2 \leq \int_{\Omega} (\partial_u f^2(u^2) - \partial_u f^2(u^1)) \cdot u.$$

With Gronwall's inequality, as  $f^2$  is Lipschitz continuous, and since  $t_0$  was arbitrary, we find  $u \equiv 0$  in  $\Omega_T$  which leads to

$$\int_{\Omega_T} \mathcal{E}(v) : C\mathcal{E}(v) = 0.$$

With Korn's inequality this yields  $v \equiv 0$  in the whole of  $\Omega_T$ . □

### 6. LOGARITHMIC FREE ENERGY

In the upcoming three sections we are going to extend Theorem 4.1 to logarithmic free energies. The results will in particular be valid for the free energy functional,

$$f(u', \mathcal{E}(v')) = k_B \theta \sum_{j=1}^n u'_j \ln u'_j + \frac{1}{2} u' \cdot Au' + W^{\text{el}}(u', \mathcal{E}(v')) \tag{6.1}$$

where  $\theta$  denotes the (fixed) temperature and  $k_B$  the Boltzmann constant. We will exploit this particular structure of  $f$  in the sequel.

As is well known the mathematical discussion is much more subtle,  $f$  becomes singular as one  $u_j$  approaches 0. To show that  $0 < u_j < 1$  for every  $j$ , we approximate  $f$  for  $\delta > 0$  by some  $f^\delta$  that fulfills the requirements of Section 2.3 and find suitable a-priori estimates that allow to pass to the limit  $\delta \rightarrow 0$ .

Despite of the mathematical difficulties, the logarithmic free energy guarantees that the vector  $u$  of order parameters lies in the transformed Gibbs simplex

$$G := \Sigma \cap \left\{ u' \in \mathbb{R}^n : u'_j \geq 0 \text{ for } 1 \leq j \leq n \text{ and } \sum_{i=1}^n u'_i = 1 \right\}$$

and is therefore physically meaningful.

The assumptions (A2) and (A3) of Section 2.3 are replaced by the following assumptions:

(A2')  $f$  is of the form (6.1), where  $A \in \mathbb{R}^{n \times n}$  is a symmetric positive definite matrix and  $\theta > 0$  the constant temperature.

(A3') The initial value  $u_0 = (u_{01}, \dots, u_{0n}) \in X_1$  fulfills  $u_0 \in G$  almost everywhere and

$$\int_{\Omega} u_{0j} > 0 \quad \text{for } 1 \leq j \leq n.$$

The other assumptions are unchanged and continue to hold.

To proceed, we define for  $d \in \mathbb{R}$  and given  $\delta > 0$  the regularised free energy functional

$$\psi^\delta(d) := \begin{cases} d \ln d & \text{for } d \geq \delta, \\ d \ln \delta - \frac{\delta}{2} + \frac{d^2}{2\delta} & \text{for } d < \delta. \end{cases}$$

The regularised free energy functional is defined in such a way that  $\psi^\delta \in C^2$  and the derivative  $(\psi^\delta)'$  is monotone. This definition goes back to the work [13] by Elliott and Luckhaus.

Due to Assumption (A2'), this leads to

$$f^\delta(u, \mathcal{E}(v')) = f^{1,\delta}(u) + f^2(u) + W^{\text{el}}(u', \mathcal{E}(v')), \quad (6.2)$$

$$f^{1,\delta}(u') := k_B \theta \sum_{j=1}^n \psi^\delta(u'_j), \quad (6.3)$$

$$f^2(u') := \frac{1}{2} u' \cdot A u'. \quad (6.4)$$

As can be easily checked,  $f^{1,\delta}, f^2$  fulfill the assumptions of Section 2.3.

**6.1. Uniform estimates.** The following lemma was first stated and proved in [13] for logarithmic free energies typical for the Cahn-Hilliard system. The proof of Elliott and Luckhaus can be directly transferred to the situation considered here with the regularised free energy defined by (6.1).

**Lemma 6.1** (Uniform bound from below on  $f^\delta$ ). *There exists a  $\delta_0 > 0$  and a  $K > 0$  such that for all  $\delta \in (0, \delta_0)$*

$$f^{1,\delta}(u) + f^2(u) \geq -K \quad \text{for all } u \in \Sigma.$$

Now we summarise the results for the regularised problem proved in Lemma 3.3 and Theorem 3.4. Lemma 6.2 also states the boundedness and convergence of the numerical solutions as  $\delta \searrow 0$ .

**Lemma 6.2** (A-priori and compactness results for regularised problem).

(a) *For all  $\delta \in (0, \delta_0)$  there exists a weak solution  $(u^\delta, v^\delta)$  of (1.4)-(1.8) with a logarithmic free energy that satisfies (A2'), (A3'), (A4)-(A6) in the sense of Section 2.1.*

(b) There exists a constant  $C > 0$  independent of  $\delta$  such that for all  $\delta \in (0, \delta_0)$

$$\sup_{t \in [0, T]} \{ \|u^\delta(t)\|_{H^1} + \|v^\delta(t)\|_{H^1} \} \leq C,$$

$$\sup_{t \in [0, T]} \int_{\Omega} f^{1, \delta}(u^\delta(t)) + \|\partial_t u^\delta\|_{L^2(\Omega_T)} \leq C,$$

$$\|u^\delta(t_2) - u^\delta(t_1)\|_{L^2} \leq C|t_2 - t_1|^{1/4} \quad \text{for all } t_1, t_2 \in [0, T].$$

(c) One can extract a subsequence  $(u^\delta)_{\delta \in \mathcal{R}}$ , where  $\mathcal{R} \subset (0, \delta_0)$  is a countable set with zero as the only accumulation point such that

- (i)  $u^\delta \rightarrow u$  in  $C^{0, \alpha}([0, T]; L^2(\Omega; \mathbb{R}^n))$  for all  $\alpha \in (0, \frac{1}{4})$ ,
- (ii)  $u^\delta \rightarrow u$  in  $L^\infty(0, T; L^2(\Omega; \mathbb{R}^n))$ ,
- (iii)  $u^\delta \rightarrow u$  almost everywhere in  $\Omega_T$ ,
- (iv)  $u^\delta \overset{*}{\rightharpoonup} u$  in  $L^\infty(0, T; H_0^1(\Omega; \mathbb{R}^n))$ ,
- (v)  $v^\delta \rightarrow v$  in  $L^2(0, T; H^1(\Omega))$

as  $\delta \in \mathcal{R}$  tends to zero.

*Proof.* Using Lemma 6.1, the regularised problem satisfies the assumptions of Section 2.3 and by Theorem 4.1, a weak solution for fixed  $\delta \in (0, \delta_0)$  exists. This proves (a). Lemma 3.3 and Theorem 3.4 imply directly (b). From Lemma 3.3 it follows that  $F^\delta(u_0, \mathcal{E}(v_0))$  does not depend on  $\delta$ , hence the constant on the right hand side does not depend on  $\delta$ . Theorem 3.4 leads to Assertion (c).  $\square$

### 7. HIGHER INTEGRABILITY FOR THE LOGARITHMIC FREE ENERGY

Since  $\varphi^\delta := (\psi^\delta)'$  will be singular as  $\delta \rightarrow 0$  we introduce for  $r > 0$

$$\varphi_r^\delta(d) := \begin{cases} \varphi^\delta(d) |\varphi^\delta(d)|^{r-1} & \text{if } \varphi^\delta(d) \neq 0, \\ 0 & \text{if } \varphi^\delta(d) = 0. \end{cases}$$

By definition,  $\varphi_r^\delta \in C^0(\mathbb{R})$ .

For  $0 < r < 1$ ,  $\varphi_r^\delta$  is not differentiable at the zero point of  $\varphi^\delta$ . To overcome this difficulty, for  $u > 0$  we introduce the function  $\varphi_r^{\delta, \varepsilon}$  with  $\varphi_r^{\delta, \varepsilon} = \varphi_r^\delta$  in  $\mathbb{R} \setminus [0, 1]$  and define  $\varphi_r^{\delta, \varepsilon}$  in  $[0, 1]$  such that  $\varphi_r^{\delta, \varepsilon}$  is a  $C^1$  function, monotone increasing and  $\varphi_r^{\delta, \varepsilon} \rightarrow \varphi_r^\delta$  in  $C^0(\mathbb{R})$  as  $\varepsilon \searrow 0$ .

First we need a regularity result on the strain tensor. The following Lemma is taken from [17] where it is also proved.

**Lemma 7.1** (Higher integrability of the strain tensor). *Suppose that  $u \in L^\sigma(\Omega, \mathbb{R}^n)$  for a  $\sigma > 2$ . Then there exists a  $p \in (2, \sigma]$  independent of  $u$  such that for all  $v \in H^1(\Omega, \mathbb{R}^n)$  which fulfill for all  $\zeta \in H^1(\Omega, \mathbb{R}^n)$  the identity*

$$\int_{\Omega} \partial_u W^{\text{el}}(u, \mathcal{E}(v)) : \nabla \zeta = \int_{\Omega} \bar{S} : \nabla \zeta$$

*the integrability property  $\nabla u \in L^p(\Omega, \mathbb{R}^{D \times D})$  holds. In particular,*

$$\|\nabla v\|_{L^p(\Omega, \mathbb{R}^{D \times D})} \leq C(\|\nabla v\|_{L^2(\Omega, \mathbb{R}^{D \times D})} + \|u\|_{L^p(\Omega, \mathbb{R}^n)} + 1)$$

*independent of  $u$ .*

Even though by construction  $0 < u_j < 1$  almost everywhere, it might still happen that for the limit the sets  $\{x \in \Omega \mid u_j(x) = 0\}$  and  $\{x \in \Omega \mid u_j(x) = 1\}$  have non-zero Lebesgue measure and that the entropic terms in the free energy density become singular. To show that this is not the case we need the following

**Lemma 7.2** (Integrability of the regularised free energy). *There exists a  $q > 1$  and a constant  $C > 0$  such that for all  $\delta \in (0, \delta_0)$*

$$\|\varphi^\delta(u_j^\delta)\|_{L^q(\Omega_T)} \leq C \quad \text{for all } 1 \leq j \leq n. \quad (7.1)$$

*Proof.* Starting point is the weak formulation (2.2)

$$\begin{aligned} & \int_{\Omega_T} k_B \theta P(\varphi^\delta(u_i^\delta))_{1 \leq i \leq n} \cdot \xi \\ &= - \int_{\Omega_T} \partial_t u^\delta \cdot \xi - \int_{\Omega_T} \gamma^2 \nabla u^\delta : \nabla \xi - \int_{\Omega_T} P A u^\delta \cdot \xi - \int_{\Omega_T} P \partial_u W^{\text{el}}(u^\delta, \mathcal{E}(v^\delta)) \cdot \xi \end{aligned} \quad (7.2)$$

which holds for all  $\xi \in L^2(0, T; H_0^1(\Omega; \mathbb{R}^n))$  with  $\partial_t \xi \in L^2(\Omega_T)$ ,  $\xi(T) = 0$ . We want to use Lemma 7.1 and notice that due to the Sobolev embedding theorem  $u^\delta \in L^\infty(0, T; L^s(\Omega))$ , where  $s = \frac{2D}{D-2}$  if  $D \geq 3$  and  $s \in [1, \infty)$  if  $D = 2$  and  $u^\delta \in L^\infty(\Omega_T)$  for  $D = 1$ . So we find  $\nabla u^\delta \in L^\infty(0, T; L^p(\Omega))$  for some  $p > 2$ . We choose  $p$  such that  $p \in (2, 4]$  and such that  $p \in (2, \frac{2D}{D-2})$  if  $D \geq 3$ . This means that also test functions  $\xi \in L^2(0, T; H^1(\Omega, \mathbb{R}^D)) \cap L^{\frac{p}{p-2}}(\Omega_T, \mathbb{R}^n)$  are allowed. So we can test (7.2) with  $\xi := [\varphi_r^{\delta, \varrho}(u_j^\delta)]_{1 \leq j \leq n}$  for  $0 < r \leq 1$ . A reformulation of the left hand side yields

$$\begin{aligned} & k_B \theta P(\varphi^\delta(u_i^\delta))_{1 \leq i \leq n} \cdot (\varphi_r^{\delta, \varrho}(u_i^\delta))_{1 \leq i \leq n} \\ &= k_B \theta \sum_{j=1}^n \left( \varphi^\delta(u_j^\delta) - \frac{1}{n} \sum_{i=1}^n \varphi^\delta(u_i^\delta) \right) \varphi_r^{\delta, \varrho}(u_j^\delta) \\ &= k_B \theta \frac{1}{n} \sum_{i,j=1}^n (\varphi^\delta(u_i^\delta) - \varphi^\delta(u_j^\delta)) \varphi_r^{\delta, \varrho}(u_i^\delta) \\ &= k_B \theta \frac{1}{n} \left[ \sum_{i < j}^n (\varphi^\delta(u_i^\delta) - \varphi^\delta(u_j^\delta)) \varphi_r^{\delta, \varrho}(u_i^\delta) + \sum_{i > j}^n (\varphi^\delta(u_i^\delta) - \varphi^\delta(u_j^\delta)) \varphi_r^{\delta, \varrho}(u_j^\delta) \right] \\ &= k_B \theta \frac{1}{n} \sum_{i < j}^n (\varphi^\delta(u_i^\delta) - \varphi^\delta(u_j^\delta)) (\varphi_r^{\delta, \varrho}(u_i^\delta) - \varphi_r^{\delta, \varrho}(u_j^\delta)). \end{aligned}$$

Due to  $(\varphi_r^{\delta, \varrho})' \geq 0$  we furthermore find

$$-\gamma^2 \int_{\Omega_T} \sum_{i=1}^n \nabla u_i^\delta \cdot \nabla \varphi_r^{\delta, \varrho}(u_i^\delta) \leq 0.$$

Using the Hölder inequality, (7.2) implies

$$\begin{aligned} & k_B \theta \frac{1}{n} \sum_{i < j}^n (\varphi^\delta(u_i^\delta) - \varphi^\delta(u_j^\delta)) (\varphi_r^{\delta, \varrho}(u_i^\delta) - \varphi_r^{\delta, \varrho}(u_j^\delta)) \\ & \leq C \left( \|\partial_t u^\delta\|_{L^2(\Omega_T)} + \|u^\delta\|_{L^2(\Omega_T)} \right) \max_{1 \leq i \leq n} \|\varphi_r^{\delta, \varrho}(u_i^\delta)\|_{L^2(\Omega_T)} \\ & \quad + C \left( \int_{\Omega_T} |\partial_u W^{\text{el}}(u^\delta, \mathcal{E}(v^\delta))|^{p/2} \right)^{\frac{2}{p}} \left( \max_{1 \leq i \leq n} \int_{\Omega_T} |\varphi_r^{\delta, \varrho}(u_i^\delta)|^{\frac{p}{p-2}} \right)^{1 - \frac{2}{p}}. \end{aligned}$$

Now we let  $\varrho \searrow 0$  and employ the estimates of Lemma 6.2 and the regularity result of Lemma 7.1. With Young's inequality we can deduce for any  $\alpha > 0$  the existence

of a constant  $C_\alpha$  with

$$k_B\theta \frac{1}{n} \sum_{i < j}^n (\varphi^\delta(u_i^\delta) - \varphi^\delta(u_j^\delta))(\varphi^\delta(u_i^\delta) - \varphi^\delta(u_j^\delta)) \leq \alpha \left( \max_{1 \leq i \leq n} \int_{\Omega_T} |\varphi^\delta(u_i^\delta)|^{\frac{p}{p-2}} \right) + C_\alpha. \tag{7.3}$$

A direct computation exploiting the monotonicity of  $\varphi^\delta$  and  $\varphi_r^{\delta,\varrho}$  finally yields

$$\frac{1}{2} \max_{1 \leq i \leq n} |\varphi^\delta(u_i^\delta)|^{1+r} \leq C \sum_{i < j} (\varphi^\delta(u_i^\delta) - \varphi^\delta(u_j^\delta)) (\varphi_r^{\delta,\varrho}(u_i^\delta) - \varphi_r^{\delta,\varrho}(u_j^\delta)).$$

This last result in combination with (7.3), after choosing  $\alpha$  sufficiently small and setting  $r = \frac{p-2}{p}$  ends the proof.  $\square$

### 8. GLOBAL EXISTENCE OF SOLUTIONS II

**Theorem 8.1** (Global existence of solutions for logarithmic free energy). *Let the assumptions of Section 6 hold. Then there exists a weak solution  $(u, v)$  in the sense of Section 2.1 of the sharp interface equations (1.4)-(1.8) with logarithmic free energy such that*

- (i)  $u \in C^{0, \frac{1}{4}}([0, T]; L^2(\Omega; \mathbb{R}^n))$ ,
- (ii)  $\partial_t u \in L^2(\Omega_T; \mathbb{R}^n)$ ,
- (iii)  $v \in L^\infty(0, T; H^1(\Omega, \mathbb{R}^D))$ ,
- (iv)  $\ln u_j \in L^1(\Omega_T)$  for  $1 \leq j \leq n$  and  $0 < u_j < 1$  almost everywhere.

*Proof.* We pass to the limit  $\delta \searrow 0$  in the weak formulation (2.2), (2.3) with  $f$  defined by (6.2) and have to show that  $(u, v)$  found in Lemma 6.2 is a solution. The limit for (2.3) can be justified in the same way as in the proof of Theorem 4.1. It remains to control the limit  $\delta \searrow 0$  in (2.2),

$$\begin{aligned} & - \int_{\Omega_T} \partial_t \xi \cdot (u^\delta - u_0) + \gamma^2 \int_{\Omega_T} \nabla u^\delta : \nabla \xi + \int_{\Omega_T} k_B \theta P(\varphi^\delta(u_i^\delta)_{1 \leq i \leq n}) \cdot \xi \\ & + \int_{\Omega_T} P(Au^\delta + \partial_u W^{\text{el}}(u^\delta, \mathcal{E}(v^\delta))) \cdot \xi = 0. \end{aligned}$$

The arguments of Theorem 4.1 can be reused except for  $k_B \theta P(\varphi^\delta(u_i^\delta)_{1 \leq i \leq n}) \cdot \xi$ .

Now we will show that  $\varphi^\delta(u_k^\delta)$  converges to  $\varphi(u_k)$  almost everywhere in  $\Omega_T$ . From the almost everywhere convergence of  $u_k^\delta$  to  $u_k$ , (7.1) and the Lemma of Fatou we find

$$\int_{\Omega_T} \liminf_{\delta \searrow 0} |\varphi^\delta(u_k^\delta)|^q \leq \liminf_{\delta \searrow 0} \int_{\Omega_T} |\varphi^\delta(u_k^\delta)| \leq C.$$

Next we show that

$$\lim_{\delta \searrow 0} \varphi^\delta(u_k^\delta) = \begin{cases} \varphi(u_k) & \text{if } \lim_{\delta \searrow 0} u_k^\delta = u_k \in (0, 1), \\ \infty & \text{if } \lim_{\delta \searrow 0} u_k^\delta = u_k \notin (0, 1) \end{cases} \tag{8.1}$$

almost everywhere in  $\Omega_T$ . For a point  $(x, t) \in \Omega_T$  with  $\lim_{\delta \searrow 0} u_k^\delta(x, t) = u_k(x, t)$  we obtain from  $\varphi^\delta(d) = \varphi(d)$  for  $d \geq \delta$  that  $\varphi^\delta(u_k^\delta(x, t)) \rightarrow \varphi(u_k(x, t))$  as  $\delta \searrow 0$ . In the second case of a point  $(x, t) \in \Omega_T$  with  $\lim_{\delta \searrow 0} u_k^\delta(x, t) = u_k(x, t) \leq 0$ , we have that for  $\delta$  small enough,

$$|\varphi^\delta(u_k^\delta(x, t))| \geq \varphi(\max\{\delta, u_k^\delta(x, t)\}) \rightarrow \infty \quad \text{for } \delta \searrow 0.$$

This proves (8.1).

From (8.1) and the higher integrability (7.1) we deduce  $0 < u_k < 1$  almost everywhere,  $\int_{\Omega_T} |\varphi(u_k)|^q \leq C$  and  $\varphi^\delta(u_k^\delta) \rightarrow \varphi(u_k)$  almost everywhere. Since  $q > 1$ , with Vitali's theorem we find

$$\varphi^\delta(u_k^\delta) \rightarrow \varphi(u_k) \quad \text{in } L^1(\Omega_T).$$

So we can pass to the limit in (2.3).  $\square$

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THOMAS BLESGEN

MAX PLANCK INSTITUTE FOR MATHEMATICS IN THE SCIENCES, INSELSTRASSE 22-26, 04103 LEIPZIG, GERMANY

*E-mail address:* blesgen@mis.mpg.de

ULRICH WEIKARD

FACULTY OF MATHEMATICS, UNIVERSITY OF DUISBURG-ESSEN, LOTHARSTRASSE 65, 47048 DUISBURG, GERMANY

*E-mail address:* wkdm@math.uni-duisburg.de