A Sharp Interface Model for Phase Transitions in Crystals with Linear Elasticity

T. Blesgen
Faculty for Mathematics and Computer Science, University of Leipzig, Augustusplatz 10/11, 04109 Leipzig, Germany, EMail: blesgen@mis.mpg.de,
Phone:+49 (341) 97-32109, FAX:+49 (341) 97-32199

U. Weikard
Faculty of Mathematics, University of Duisburg-Essen, Lotharstr. 65, 47048 Duisburg, Germany, EMail: wkd@math.uni-duisburg.de,
Phone:+49 (203) 379 4049

Abstract:
A model describing phase transitions coupled with diffusion and linear elasticity in crystals under isothermal conditions is introduced. The elastic deformation as well as the phase parameter are obtained directly by the minimisation of the free energy. After stating the model, the existence of strong solutions is proved.

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1 Introduction

The model introduced here represents a crystal for fixed temperature where n different species of molecules diffuse and where two phases may coexist. The elastic behaviour is described by a linear approximation. The model is related to the Stefan model but allows for deformation and considers an isothermal setting without diffusion of latent heat. For a survey of results on the Stefan problem see [1], [2]. The present article is part of a larger program to bring forward the understanding of mechanics of multi-phase structures in solids. In [3] the case of non-linear deformations is analysed imposing suitable growth conditions on the gradient of the deformation. The techniques in [3] are fully non-linear and exclude the case of linear elasticity treated here. In [4] the model of this article is studied numerically in two space dimensions making use of a level set method to find the local minimum of the free energy w.r.t. the phase parameter.

The existence result shown in Section 9 will in particular imply that even though the density function may jump across a phase transition the chemical potential remains a smooth function. This allows to set up jump conditions and is crucial for the numerical treatment of the model. The structure of the existence proof persued in this paper follows [5]. The main modifications arise from the additional formulation as a minimum in the phase parameter, see Equation (10) below, and from the fact that no regularising gradient term of the concentration vector occurs. The general outline of the approach is related to the earlier work [6]. The idea of approximation by a discrete scheme and showing compactness in time is classical and goes back to Leray, [7].

This work is organised in the following way. In Section 2 the model is derived and the physical assumptions for the validity of the model are listed. Section 3 provides the necessary notations and function spaces.

Starting from the time-discrete solution, uniform bounds are derived and the discrete solution is extended by linear interpolation. This is first done for polynomial free energies f_l and the existence of global solutions in Section 9 is only valid for polynomial f_l. Using these results, in Sections 10 to 12 the existence proof is extended to logarithmic free energies that become singular as the density of one component approaches 0 or 1.

2 Derivation of the Model

Let $\Omega \subset \mathbb{R}^D$, $1 \leq D \leq 3$ be the bounded domain of reference, $\Phi : \mathbb{R}^D \times \mathbb{R}_{\geq 0} \longrightarrow \mathbb{R}^D$ a deformation. $\Phi(\Omega, t)$ defines the crystal at time t, $x \in \Omega$ are the Lagrange coordinates.

Instead of Φ we will use the displacement vector u, where

$$\Phi(t) = \mathrm{Id} + u(t).$$

$\Omega = \Phi(\Omega, 0)$ is the unstrained body, which goes along with $u(t = 0) = 0$.

The particle densities of the n different species of molecules are determined by $\varrho_i = \varrho_i(x,t)$. Let $\varrho := (\varrho_1, \ldots, \varrho_n)$. The densities fulfil for $1 \leq i \leq n$

$$\varrho_i \geq 0, \varrho_i \in H^{1,2}(\Omega), \int_\Omega \varrho_i(x,t)\,dx = \int_\Omega \varrho_{i_0}(x)\,dx$$

with given initial values ϱ_{i_0} and, due to the possible presense of vacancies,

$$\sum_{i=1}^n \varrho_i \leq 1.$$

This reflects the possibility that some positions in the lattice crystal are not occupied by particles.

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. $\|\cdot\|_{H^{1,2}(\Omega)}$ and by $BV(\Omega)$ the space of functions with bounded variation, see for instance [8]. By $\|\cdot\|_{H^1}$ and $\|\cdot\|_{BV}$ we always mean $\|\cdot\|_{H^{1,2}(\Omega)}$ and $\|\cdot\|_{BV(\Omega)}$. $C_0^\infty(\Omega) := \cap_{m=0}^\infty C_0^m(\Omega)$ where $C_0^m(\Omega)$ is the space of m-times continuously differentiable functions over Ω with compact support.

Since we are concerned with two-phase structures we introduce $\chi = \chi(\cdot, t) \in X_2$, where

$$X_2 := \{\chi' \in BV(\Omega) \,|\, \chi'(1-\chi') = 0 \text{ almost everywhere in } \Omega\}.$$

$f_j = f_j(\varrho, u)$ denotes the free energy density of phase j, $j = 1,2$. f_j are smooth functions and convex in ϱ; possible examples are

$$f_j(\varrho, u) := \frac{1}{2}(\varrho - \overline{\varrho}_j)^2 + W^{\mathrm{el}}(\varrho, u), \tag{1}$$

$$f_j(\varrho, u) := \alpha_j \sum_{i=1}^n \varrho_i \ln \varrho_i + W^{\mathrm{el}}(\varrho, u). \tag{2}$$

The coefficients α_j will in general depend on temperature T which is kept constant here. W^{el} in (1), (2) is the elastic energy density, i.e. the contribution of the deformation to the free energy. It was first studied by Eshelby, [9].

W^{el} can by Hooke's law be computed to

$$W^{\mathrm{el}}(\varrho, u) := \frac{1}{2}(\mathcal{E}(u) - \overline{\varepsilon}(\varrho)) : C(\varrho)(\mathcal{E}(u) - \overline{\varepsilon}(\varrho)), \tag{3}$$

where

$$\mathcal{E} = \mathcal{E}(u) = \mathcal{E}_{ij}(u) := \frac{1}{2}(\partial_i u_j + \partial_j u_i)$$

is the elasticity tensor. If e denotes the lattice misfit we assume the linear relationship (*Vegard's law*)

$$\overline{\varepsilon}(\varrho) := e\varrho\,\mathrm{Id}. \tag{4}$$

$C(\varrho)$ is the elasticity tensor that maps symmetric tensors in $\mathbb{R}^{D\times D}$ onto itself. We assume that C is symmetric, positive definite and does not depend on χ. $\overline{\varepsilon}(\varrho)$ is the eigenstrain at density ϱ. Under the assumptions that lead to Equation (4) the eigenstrain $\overline{\varepsilon}$ is uniquely defined.

Since the system free energy density f is the convex hull of f_1, f_2, we define f as the convex combination

$$f = \chi f_1 + (1 - \chi) f_2.$$

The interfacial surface energy for given surface tension $\sigma > 0$ is

$$F_S(\chi(t)) = \sigma \int_\Omega |\nabla\chi(x,t)|\, dx.$$

Thus, if the surface energy is bounded the total variation of χ in Ω is bounded, too. The term

$$F^{\mathrm{out}}(u) := \int_\Omega \overline{W}(\mathcal{E}(u))$$

represents energy effects due to applied outer forces. We assume that there are no 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. The work necessary to transform $\Omega = \Phi(\Omega, 0)$ to $\Phi(\Omega, t)$ with corresponding displacement vector $u(t)$ is therefore

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

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

The deformation in the non-linear model [3] is computed by taking the infimum of f over all allowed deformations. In the case of linear elasticity we can simplify this. The displacement u is obtained by solving the elliptic equation

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

with the stress tensor

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

So the system free energy obeys the formula

$$F(\varrho(t),\chi(t),u(t)) = F_S(\chi(t))+F^{\text{out}}(u(t))+\int\limits_{\Omega} \chi(t)f_1(\varrho(t),u(t))+(1-\chi(t))f_2(\varrho(t),u(t))\,dx. \quad (5)$$

The diffusive flow is caused by the gradient of the chemical potentials. By Onsager's law, the flux J is given by

$$J(t) = L\nabla\mu(t)$$

where $\nabla\mu := (\nabla\mu_1,\dots,\nabla\mu_n)$ and L is the $n\times n$ mobility tensor. L is positive semi-definite, but in order to avoid degenerate cases we will assume in the sequel that L is positive definite.

Hence, for a given stop time $T_0 > 0$ we end up with the following model:

Find for $t \geq 0$ the vector (ϱ,χ,μ,u) such that in $\Omega_{T_0} := \Omega\times(0,T_0)$

$$\begin{aligned}
\partial_t\varrho &= \operatorname{div}(L\nabla\mu), && (6)\\
\mu &= \frac{\partial f}{\partial\varrho}, && (7)\\
\operatorname{div}(S) &= 0, && (8)\\
S &= \partial_\varepsilon W^{el}(\varrho,\mathcal{E}(u)), && (9)\\
F(\varrho(t),\chi(t),u(t)) &= \min_{\tilde\chi\in X_2} F(\varrho(t),\tilde\chi,u(t)) && (10)
\end{aligned}$$

with the initial data for $t=0$ in Ω

$$\varrho(\cdot,0) = \varrho_0(\cdot) \quad (11)$$

and for $t>0$ in $\partial\Omega$

$$\varrho=\varrho_d, \mu=\mu_d, \qquad S\vec n = \overline{S}\vec n. \quad (12)$$

Remarks:

- Instead of the Dirichlet boundary condition on ϱ and μ, other conditions as Neumann conditions or periodic conditions are as well possible in (12).
- Equation (10) does not control the variation of χ in time.
- In other models an evolution equation like

$$\tau\partial_t\chi = -\frac{\partial F}{\partial\chi}(\varrho,\chi,u)$$

  for a given constant $\tau>0$ governs χ. If we compare this with the above model, we find that Equation (10) means that the phase parameter adapts instantaneously.
- Simple examples show that the solutions of (6)–(12) are in general not unique due to an ambiguity in χ.
- The existence of a minimum in Equation (10) w.r.t. χ is guaranteed by the Poincaré inequality and the term $\sigma|\nabla\chi|$.

3 Preliminaries to the existence proof

In the remaining sections we discuss the existence theory to the sharp interface model (6)-(12). We will show that under suitable growth conditions on the free energy density, collected in Section 6 and for logarithmic energies in Section 10, discrete solutions to the implicit time discretisation exist. A priori estimates allow to pass to the limit and show the existence of solutions to the model with polynomial free energy. This result is then used to generalise to the sharp interface model with logarithmic free energy.

We will carry out the proof for classical Dirichlet boundary data, i.e. set w.l.o.g. $\varrho_d = \mu_d = 0$ in (12). If the general Dirichlet condition $\varrho = \varrho_d$ on $\partial\Omega$ is imposed, one can formally set $\tilde{\varrho} := \varrho - \varrho_d$ and gain from the results for $\tilde{\varrho}$ provided in Theorem 2 directly the corresponding statements for ϱ. Other boundary conditions will be 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 concentration vector ϱ lies inside the simplex Σ,

$$\varrho \in \Sigma := \Big\{ \varrho' = (\varrho'_1, \dots, \varrho'_n) \in \mathbb{R}^n \;\Big|\; \sum_{i=1}^n \varrho'_i = 1 \Big\}.$$

Notice that the condition $0 \le \varrho_i \le 1$ in Ω may be violated for polynomial free energies considered in the first part of this article. Let

$$\begin{aligned} X_1 &:= \{\varrho' \in L^2(\Omega;\mathbb{R}^n) \mid \varrho' \in \Sigma \text{ almost everywhere in } \Omega\}, \\ X_3 &:= \{u' \in H^1(\Omega,\mathbb{R}^D) \,|\, (u',v)_{H^1} = 0 \text{ for all } v \in X_{\text{ird}}\}, \end{aligned}$$

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

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

Let us now consider the mapping $\mathcal{L}(\mu) : Y \to \mathcal{D}$ corresponding to $\mu \mapsto -\text{div}(L\nabla\mu)$ with Dirichlet boundary conditions, defined by

$$\mathcal{L}(\mu)(\zeta) := \int_\Omega L\nabla\mu : \nabla\zeta.$$

To simplify the further argumentation we will introduce the inverse $\mathcal{G}$ of $\mathcal{L}$. The existence of $\mathcal{G}$ is derived from the Poincaré inequality and the Lax-Milgram theorem, since L is positive definite. From this we find that $\mathcal{G}$ is positive definite, self-adjoint, injective and compact.

Hence, we have

$$(L\nabla\mathcal{G}v, \nabla\zeta)_{L^2} = (\zeta, v) \quad \text{for all } \zeta \in Y \text{ and } v \in \mathcal{D}.$$

Since L is positive definite, we define for $v_1, v_2 \in \mathcal{D}$ the L scalar product

$$(v_1, v_2)_L := (L\nabla\mathcal{G}v_1, \nabla\mathcal{G}v_2)_{L^2}$$

and the corresponding norm

$$\|v\|_L := \sqrt{(v,v)_L}.$$

Functions $v \in Y$ canonically define an element in $\mathcal{D}$ and consequently, $(\cdot,\cdot)_L$ and $\|\cdot\|_L$ are also well-defined for elements in Y.

The Green's function $\mathcal{G}$ allows to rewrite the conservation of mass equation (6) as

$$\mathcal{G}\partial_t\varrho = \mu = \Big(\frac{\partial f}{\partial \varrho_j}\Big)_{1\le j\le n}. \tag{13}$$

Remark: If we replace the Dirichlet conditions for ϱ and μ by a Neumann boundary condition or periodic boundary conditions, a (generalised) Poincaré inequality holds in $H^{1,2}(\Omega)$. For instance in case of periodic boundary conditions the inverse $\mathcal{G}$ of $\mathcal{L}$ (now defined with periodicity condition) exists and the above construction as well as all the results found below continue to hold.

4 The weak formulation

The vector $(\varrho,\chi,\mu,u) \in L^2(\Omega_{T_0};\ \mathbb{R}^n) \times BV(\Omega_{T_0}) \times L^2(0,T_0;\ H_0^{1,2}(\Omega;\mathbb{R}^n)) \times L^2(0,T_0;\ X_3)$ is called a *weak solution of* (6)-(12) if

$$-\int\limits_{\Omega_{T_0}} \partial_t\xi\cdot(\varrho-\varrho_0) + \int\limits_{\Omega_{T_0}} L\nabla\mu : \nabla\xi = 0 \tag{14}$$

for all $\xi \in L^2(0,T_0;\ H_0^1(\Omega;\mathbb{R}^n))$ with $\partial_t\xi \in L^2(\Omega_{T_0})$, $\xi(T_0)=0$, and

$$\int\limits_{\Omega_{T_0}} \mu\cdot\zeta = \int\limits_{\Omega_{T_0}} \frac{\partial f}{\partial\varrho}(\varrho,\chi,u)\cdot\zeta \tag{15}$$

for all $\zeta \in L^2(\Omega_{T_0};\ \mathbb{R}^n)$, and

$$\int\limits_{\Omega_{T_0}} W^{\mathrm{el}}(\varrho,\mathcal{E}(u)) : \nabla\eta = \int\limits_{\Omega_{T_0}} \overline{S} : \nabla\eta \tag{16}$$

for all $\eta \in L^2(0,T_0;\ H^1(\Omega;\mathbb{R}^n))$ and if for all $t\in[0,T_0]$

$$F(\varrho(t),\chi(t),u(t)) = \min_{\tilde\chi\in X_2} F(\varrho(t),\tilde\chi,u(t)). \tag{17}$$

5 The implicit time discretisation

We fix an $M\in\mathbb{N}$ and set $h := \frac{T_0}{M}$. For $m\ge 1$ and given ϱ^{m-1} consider

$$\frac{\varrho^m-\varrho^{m-1}}{h} = \operatorname{div}(L\nabla\mu^m), \tag{18}$$

$$\mu^m = \frac{\partial f}{\partial\varrho}(\varrho^m,\chi^m,u^m), \tag{19}$$

$$\operatorname{div}(S^m) = 0, \tag{20}$$

$$S^m = \partial_\varepsilon W^{\mathrm{el}}(\varrho^m,\mathcal{E}^m), \tag{21}$$

$$F(\varrho^m,\chi^m,u^m) = \min_{\tilde\chi\in X_2} F(\varrho^m,\tilde\chi,u^m). \tag{22}$$

6 Structural Assumptions

In order to be able to establish the existence of weak solutions in the sense of Section 4, 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

$$f(\varrho, \chi, u) = \bar{f}(\varrho, \chi) + W^{el}(\varrho, \mathcal{E}(u)) \text{ for all } \varrho \in \mathbb{R}^n,\ \chi \in \mathbb{R},\ u \in \mathbb{R}^D$$

with $\bar{f} \in C^1(\mathbb{R}^n \times \mathbb{R}; \mathbb{R})$ for every $\chi \in [0,1]$ and $\bar{f}(\cdot, \chi)$ is convex for every $\chi \in [0,1]$. Additionally we postulate

(A2.1) $\bar{f} \geq 0$.

(A2.2) There exist constants $C_1 > 0$, $C_2 \geq 0$ such that

$$C_1|\varrho|^2 - C_2 \leq \bar{f}(\varrho, \chi) \qquad \text{for all } \varrho \in \Sigma,\ \chi \in [0,1].$$

(A2.3) For all $\delta > 0$ there exists a constant $C_\delta > 0$ such that

$$|\partial_\varrho \bar{f}(\varrho, \chi)| \leq \delta \bar{f}(\varrho, \chi) + C_\delta \quad \text{for all } \varrho \in \Sigma,\ \chi \in [0,1].$$

(A3) The initial datum ϱ_0 fulfils

$$f(\varrho_0, \chi_0, u_0) < \infty,$$

where u_0 is the solution of (16) and $\chi_0 \in X_2$ the minimum in Equation (17).

(A4.1) The diffusion tensor L is assumed to be symmetric and positive definite.

(A4.2) The surface tension $\sigma > 0$ is a constant.

(A5) The elastic energy density $W^{\mathrm{el}} \in C^1(\mathbb{R}^n \times \mathbb{R}^{D\times D}; \mathbb{R})$ satisfies

(A5.1) $W^{\mathrm{el}}(\varrho', \mathcal{E}')$ only depends on the symmetric part of $\mathcal{E}' \in \mathbb{R}^{D\times D}$, i.e. $W^{\mathrm{el}}(\varrho', \mathcal{E}') = W^{\mathrm{el}}(\varrho', (\mathcal{E}')^t)$ for all $\varrho' \in \mathbb{R}^n$ and $\mathcal{E}' \in \mathbb{R}^{D\times D}$.

(A5.2) $\partial_\varepsilon W^{\mathrm{el}}(\varrho', \cdot)$ is strongly monotone uniformly in ϱ', i.e. there exists a $c_1 > 0$ such that for all symmetric $\mathcal{E}_1'$, $\mathcal{E}_2' \in \mathbb{R}^{D\times D}$

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

(A5.3) There exists a constant $C_3 > 0$ such that for all $\varrho' \in \Sigma$ and all symmetric $\mathcal{E}' \in \mathbb{R}^{D\times D}$

$$\begin{aligned} |W^{\mathrm{el}}(\varrho', \mathcal{E}')| &\leq C_3(|\mathcal{E}'|^2 + |\varrho'|^2 + 1), \\ |\partial_\varrho W^{\mathrm{el}}(\varrho', \mathcal{E}')| &\leq C_3(|\mathcal{E}'|^2 + |\varrho'|^2 + 1), \\ |\partial_\varepsilon W^{\mathrm{el}}(\varrho', \mathcal{E}')| &\leq C_3(|\mathcal{E}'| + |\varrho'| + 1). \end{aligned}$$

(A6) The energy density of the applied outer forces is of the form $\overline{W}(\mathcal{E}') = -\mathcal{E}' : \overline{S}$ with a constant symmetric tensor $\overline{S}$.

The decomposition of f in (A2) exploits the fact that the elastic energy is the same in both phases and hence does not depend on χ.

The assumptions on f are in particular valid for the case that is most interesting to us, namely

$$\bar{f}(\varrho, \chi) := \chi \tilde{f}_1(\varrho) + (1-\chi)\tilde{f}_2(\varrho),$$

where $\tilde{f}_j$ is the free energy density of phase j without the elastic and interaction terms, i.e. for the polynomial choice (1)

$$\tilde{f}_j(\varrho) := \frac{1}{2}(\varrho - \overline{\varrho}_j)^2, \quad j = 1, 2.$$

From now on we assume that the assumptions (A1)-(A6) hold.

7 Existence of solutions to the time discrete scheme

For each time step $m \geq 1$ in the implicit time discretisation (18)-(22), given time step size $h > 0$, and given ϱ^{m-1} we define the discrete energy functional

$$F^{m,h}(\varrho, \chi, u) := F(\varrho, \chi, u) + \frac{1}{2h}\|\varrho - \varrho^{m-1}\|_L^2.$$

Lemma 1: *(Existence of a minimiser)*
For $\varrho^{m-1} \in X_1$ given and any $h > 0$, the functional $F^{m,h}$ possesses a minimiser (ϱ^m, χ^m, u^m) in $X_1 \times X_2 \times X_3$.

Proof: The proof is an application of the direct method in the calculus of variations. The term $\int_\Omega \sigma|\nabla\chi|$ in the definition of F guarantees the coercivity of F for $\chi \in X_2$ and similarly $\int_\Omega W^{el}$ the coercivity of F for $u \in X_3$. Using Estimate (A2.2), we find that the functional $F^{m,h}$ is weakly lower semicontinuous and coercive in $X_1 \times X_2 \times X_3$ and hence possesses a minimiser. By construction, the minimiser χ^m of $F^{m,h}$ w.r.t. χ is at the same time a solution to (17) for $t = mh$. □

The following lemma shows that the energy functional $F^{m,h}$ is the correct one and corresponds to the implicit time discretisation (18)-(22).

Lemma 2: *(Euler-Lagrange equations)*
The minimiser (ϱ^m, χ^m, u^m) of $F^{m,h}$ fulfils

$$\int_\Omega \frac{\varrho^m - \varrho^{m-1}}{h} \cdot \xi + \int_\Omega L\nabla\mu^m : \nabla\xi = 0 \quad \textit{for all } \xi \in Y, \tag{23}$$

$$\int_\Omega \partial_\varrho f(\varrho^m, \chi^m) \cdot \zeta = \int_\Omega \mu^m \cdot \zeta \quad \textit{for all } \zeta \in Y \cap L^\infty(\Omega; \mathbb{R}^n), \tag{24}$$

$$\int_\Omega \partial_\varepsilon W^{el}(\varrho^m, \mathcal{E}(u^m)) : \nabla\eta = \int_\Omega \overline{S} : \nabla\eta \quad \textit{for all } \eta \in H^1(\Omega, \mathbb{R}^D). \tag{25}$$

Here, $\mu^m = \mathcal{G}\Big(\frac{\varrho^m - \varrho^{m-1}}{h}\Big)$.

Proof: We choose directions $\xi \in Y \cap L^\infty(\Omega; \mathbb{R}^n)$, $\zeta \in X_3 \cap L^\infty(\Omega; \mathbb{R})$ and determine the variations of $F^{m,h}(\varrho, \chi, u)$ with respect to ϱ and u for ξ, ζ. The variation w.r.t. ϱ is

$$\lim_{s\to 0}\Big((F^{m,h}(\varrho^m + s\xi, \chi^m, u^m) - F^{m,h}(\varrho^m, \chi^m, u^m))s^{-1}\Big). \tag{26}$$

Since $\varrho \mapsto \bar{f}(\varrho, \chi)$ is convex for arbitrary χ, we have

$$\bar{f}(\varrho^m, \chi^m) \geq \bar{f}(\varrho^m + s\xi, \chi^m) - s\partial_\varrho \bar{f}(\varrho^m + s\zeta, \chi^m) \cdot \xi.$$

This implies

$$\begin{aligned} \bar{f}(\varrho^m + s\xi, \chi^m) &\leq \bar{f}(\varrho^m, \chi^m) + |s\partial_\varrho \bar{f}(\varrho^m + s\xi, \chi^m)|\,\|\xi\|_{L^\infty} \\ &\leq \bar{f}(\varrho^m, \chi^m) + |s|\,\bar{f}(\varrho^m + s\xi, \chi^m)\,\|\xi\|_{L^\infty} + C|s|. \end{aligned}$$

The last is by Assumption (A2.3) with $\delta = 1$. Hence, for s small enough, we find

$$\Big|\frac{\bar f(\varrho^m + s\xi, \chi^m) - \bar f(\varrho^m, \chi^m)}{s}\Big| \le C(\bar f(\varrho^m, \chi^m) + 1).$$

Lebesgue's dominated convergence theorem implies

$$\lim_{s\to 0} \frac{1}{s}\Big(\int_\Omega f(\varrho^m + s\xi, \chi^m) - f(\varrho^m, \chi^m)\Big) = \int_\Omega \partial_\varrho f(\varrho^m, \chi^m)\cdot \xi.$$

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

$$\begin{aligned}&\lim_{s\to 0}\Big(s^{-1}(2h)^{-1}\left(\|\varrho^m + s\xi - \varrho^{m-1}\|_L^2 - \|\varrho^m - \varrho^{m-1}\|_L^2\right)\Big)\\ &\quad= \Big(\frac{\varrho^m - \varrho^{m-1}}{h}, \xi\Big)_L = \Big(\mathcal{G}\Big(\frac{\varrho^m - \varrho^{m-1}}{h}\Big), \xi\Big)_{L^2} = \Big(\mu^m, \xi\Big)_{L^2}.\end{aligned}$$

The equality (24) follows because (ϱ^m, χ^m, u^m) is a minimiser and thus the limit in (26) is 0. (23) follows from the defintion of μ^m. To derive (25), we vary $F^{m,h}$ w.r.t. u. From the symmetry of $\partial_\varepsilon W^{el}$ and $\overline{S}$ we find (25). □

8 Uniform estimates

In the preceeding section we proved the existence of a discrete solution $(\varrho^m, \mu^m, \chi^m, u^m)$ for $1 \le m \le M$ and arbitrary $M \in \mathbb{N}$. We define the piecewise constant extension $(\varrho_M, \mu_M, \chi_M, u_M)$ of $(\varrho^m, \mu^m, \chi^m, u^m)_{1\le m\le M}$ by

$$(\varrho_M(t), \mu_M(t), \chi_M(t), u_M(t)) := (\varrho_M^m, \mu_M^m, \chi_M^m, u_M^m) := (\varrho^m, \mu^m, \chi^m, u^m) \text{ for } t \in ((m-1)h, mh]$$

and $\varrho_M(0) = \varrho_0$, $\chi_M(0)$ given by Equation (22), $\mu_M(0)$ given by Equation (19) and $u_M(0)$ given by Equation (20).

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

$$(\overline{\varrho}_M, \overline{\mu}_M, \overline{\chi}_M, u_M)(t) := \beta(\varrho_M^m, \mu_M^m, \chi_M^m, u_M^m) + (1-\beta)(\varrho_M^{m-1}, \mu_M^{m-1}, \chi_M^{m-1}, u_M^{m-1}).$$

Lemma 3: *(A-priori estimates)*
The following a-priori estimates are valid.

(a) For all $M \in \mathbb{N}$ and all $t \in [0, T_0]$ we have the dissipation inequality

$$F(\varrho_M, \chi_M, u_M)(t) + \frac{1}{2}\int_{\Omega_t} L\nabla\mu_M : \nabla\mu_M \le F(\varrho_0, \chi_0, u_0).$$

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

$$\sup_{0\le t\le T_0}\Big\{\|\varrho_M(t)\|_{L^2} + \|\chi_M(t)\|_{BV} + \|u_M(t)\|_{H^1}\Big\} \;\le\; C, \tag{27}$$

$$\sup_{0\le t\le T_0}\int_\Omega \bar f(\varrho_M(t), \chi_M(t)) + \|\nabla\mu_M\|_{L^2(\Omega_{T_0})} \;\le\; C. \tag{28}$$

Proof: Since (ϱ^m, χ^m, u^m) is a minimiser of $F^{m,h}$, we have for every $m \geq 1$

$$F(\varrho^m, \chi^m, u^m) + \frac{1}{2h}\|\varrho^m - \varrho^{m-1}\|_L^2 \leq F(\varrho^{m-1}, \chi^{m-1}, u^{m-1}) \tag{29}$$

and by a direct calculation

$$\frac{1}{2h}\|\varrho^m - \varrho^{m-1}\|_L^2 = \frac{h}{2}(\nabla\mu^m, L\nabla\mu^m)_{L^2}. \tag{30}$$

When iterating (29), Equation (30) yields

$$F(\varrho_M^m, \chi_M^m, u_M^m) + \frac{1}{2}\int_0^{mh}(\nabla\mu_M^m, L\nabla\mu_M^m)_{L^2}\,dt \leq F(\varrho_0, \chi_0, u_0).$$

Using the assumptions, in particular (A2.2) to get an L^2-bound on ϱ_M, and with the help of Korn's inequality this proves the lemma. □

For the linear interpolation $\overline{\varrho}_M$ of ϱ_M^m, the Euler-Lagrange equation (23) can be rewritten as

$$\int_\Omega \partial_t\overline{\varrho}_M(t)\cdot\xi + \int_\Omega L\nabla\mu_M(t) : \nabla\xi = 0 \text{ for all } \xi \in Y \tag{31}$$

which holds for almost all $t \in (0, T_0)$. Equation (31) controls the variation of $\overline{\varrho}_M$ in time and, together with the uniform estimates of Lemma 3, allows to show compactness in time.

The following theorem is the first main result and states the convergence of the solution of the time-discretized problem. In the next part we will show that the limit is in fact a solution to (6)-(12).

Theorem 1: *(Compactness for $(\varrho_M, \mu_M, \chi_M, u_M)$)*
There exists a constant $C > 0$ such that for all $t_1, t_2 \in [0, T_0]$

$$\|\overline{\varrho}_M(t_2) - \overline{\varrho}_M(t_1)\|_{L^2} \leq C|t_2 - t_1|^{\frac{1}{4}}.$$

Furthermore, there are subsequences $(\varrho_M)_{M\in\mathcal{N}}$, $(\mu_M)_{M\in\mathcal{N}}$, $(\chi_M)_{M\in\mathcal{N}}$ and $(u_M)_{M\in\mathcal{N}}$, with $\mathcal{N} \subset \mathbb{N}$ and there are $\varrho \in L^\infty(0, T_0; L^2(\Omega))$, $\mu \in L^2(0, T_0; Y)$, $\chi \in L^\infty(0, T_0; BV(\Omega))$ and $u \in L^\infty(0, T_0; H^1(\Omega))$ such that

(i)	$\overline{\varrho}_M$	$\to$	ϱ *in* $C^{0,\alpha}([0, T_0]; L^2(\Omega; \mathbb{R}^n))$ *for all* $\alpha \in (0, \frac{1}{4})$,
(ii)	ϱ_M	$\to$	ϱ *in* $L^\infty(0, T_0; L^2(\Omega; \mathbb{R}^n))$,
(iii)	ϱ_M	$\to$	ϱ *almost everywhere in* Ω_{T_0},
(iv)	ϱ_M	$\overset{*}{\rightharpoonup}$	ϱ *in* $L^\infty(0, T_0; L^2(\Omega; \mathbb{R}^n))$,
(v)	μ_M	$\rightharpoonup$	μ *in* $L^2(0, T_0; H_0^1(\Omega; \mathbb{R}^n))$,
(vi)	u_M	$\to$	u *in* $L^2(0, T_0; H^1(\Omega))$,
(vii)	χ_M	$\to$	χ *almost everywhere in* Ω_{T_0},
(viii)	χ_M	$\to$	χ *in* $L^\infty(0, T_0; BV(\Omega))$, *with* $\chi(1-\chi) = 0$ *a.e. in* Ω,
(ix)	$\partial_\varrho\bar{f}(\varrho_M, \chi_M)$	$\to$	$\partial_\varrho\bar{f}(\varrho, \chi)$ *in* $L^1(\Omega_{T_0})$

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

Proof: We test Equation (31) with $\xi := \overline{\varrho}_M(t_2) - \overline{\varrho}_M(t_1)$, where $t_1, t_2 \in [0, T_0]$ with $t_1 < t_2$. After integration in time from t_1 to t_2, we obtain

$$\|\overline{\varrho}_M(t_2) - \overline{\varrho}_M(t_1)\|_{L^2}^2 + \int_{t_1}^{t_2} \int_\Omega L\nabla\mu_M(t) : \nabla(\overline{\varrho}_M(t_2) - \overline{\varrho}_M(t_1))\, dt = 0.$$

The ϱ_M^m are uniformly bounded in $L^2(\Omega; \mathbb{R}^n)$, therefore the linear interpolants $\overline{\varrho}_M$ are uniformly bounded in $L^\infty(0, T_0; L^2(\Omega))$. Thus we obtain

$$\begin{aligned} \|\overline{\varrho}_M(t_2) - \overline{\varrho}_M(t_1)\|_{L^2}^2 &\leq C\|\overline{\varrho}_M\|_{L^\infty(L^2)} \int_{t_1}^{t_2} \|\nabla\mu_M(t)\|_{L^2}\, dt \\ &\leq C\|\overline{\varrho}_M\|_{L^\infty(L^2)}\, (t_2 - t_1)^{\frac{1}{2}} \|\nabla\mu\|_{L^2(\Omega_{T_0})}. \end{aligned}$$

Employing the a-priori estimates (27) and (28) we have proved

$$\|\overline{\varrho}_M(t_2) - \overline{\varrho}_M(t_1)\|_{L^2} \leq C|t_2 - t_1|^{\frac{1}{4}} \text{ for all } t_1, t_2 \in [0, T_0]$$

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

The boundedness of $(\overline{\varrho}_M)$ in $L^\infty(0, T_0; L^2(\Omega))$ yields as a consequence of the Arzelà-Ascoli theorem statement (i).

The claims (ii),(iii) and (iv) are shown as follows. Choose for $t \in [0, T_0]$ 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 $\overline{\varrho}$ we get at once

$$\begin{aligned} \|\overline{\varrho}_M(t) - \varrho_M(t)\|_{L^2} &= \|\beta\varrho_M^m + (1 - \beta)\varrho_M^{m-1} - \varrho_M^m\|_{L^2} \\ &= (1 - \beta)\|\varrho_M^m - \varrho_M^{m-1}\|_{L^2} \\ &\leq Ch^{\frac{1}{4}}. \end{aligned}$$

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 (27) which gives the boundedness of ϱ_M in $L^\infty(0, T_0; L^2(\Omega; \mathbb{R}^n))$.

For the proof of (v) we notice that due to estimate (28), the $(\nabla\mu_M)$ are uniformly bounded in $L^2(\Omega_{T_0})$. By the Poincaré inequality (μ_M) are in fact uniformly bounded in $L^2(0, T_0; H_0^1(\Omega))$. With the Banach-Alaoglu theorem (v) follows.

The proof of (vi) is contained in [5], Lemma 3.5 (no $H^{1,2}$-regularity of $\varrho(\cdot, t)$ is needed).

To prove (vii), fix $t \in [0, T_0]$. The sequence $\chi_M(\cdot, t) \subset BV(\Omega)$ is uniformly bounded in $BV(\Omega)$ and from the compact imbedding $BV(\Omega) \hookrightarrow L^1(\Omega)$ we infer the existence of a subsequence $\mathcal{N}$ with $\chi_\mathcal{N}(\cdot, t) \to \chi(\cdot, t)$ in $L^1(\Omega)$. If $\varphi \in C_0^\infty(\Omega)$, then for $1 \leq i \leq n$

$$\lim_{\mathcal{N}\to\infty} \int_\Omega \varphi D_i \chi_\mathcal{N}(\cdot, t) = -\lim_{\mathcal{N}\to\infty} \int_\Omega \chi_\mathcal{N}(\cdot, t) D_i\varphi = \int_\Omega \chi(\cdot, t) D_i\varphi$$

and furthermore

$$\Big|\int_\Omega \chi(\cdot, t) D_i\varphi\Big| \leq \sup_{x\in\Omega} |\varphi(x)| \liminf_{\mathcal{N}\to\infty} \int_\Omega |\nabla\chi_\mathcal{N}(\cdot, t)| < \infty.$$

Hence, $\chi(\cdot, t) \in BV(\Omega)$ and $\chi_\mathcal{N} \to \chi$ in $L^\infty(0, T_0; BV(\Omega))$. Since in particular $\chi_\mathcal{N} \to \chi$ in $L^1(\Omega_{T_0})$, we conclude $\chi_\mathcal{N} \to \chi$ almost everywhere in Ω_{T_0} for a subsequence $\mathcal{N}$. This proves (vii). From the pointwise limit we get $\chi \geq 0$ and $\chi(1 - \chi) = 0$ almost everywhere in Ω, hence (viii).

In order to prove (ix), we first notice that by Assumption (A2), $\partial_\varrho \bar{f}$ is a continuous function. Hence, by (iii) and (vii),

$$\partial_\varrho \bar{f}(\varrho_M, \chi_M) \to \partial_\varrho \bar{f}(\varrho, \chi) \text{ almost everywhere in } \Omega_{T_0}.$$

The growth condition of Assumption (A2.3) on $\bar{f}$ now yields that for arbitrary $\delta > 0$ and all measurable $E \subset \Omega$

$$\int_E |\partial_\varrho \bar{f}(\varrho_M, \chi_M)| \le \delta \int_E \bar{f}(\varrho_M, \chi_M) + C_\delta |E| \le \delta C + C_\delta |E|.$$

Therefore, $\int_E |\partial_\varrho \bar{f}(\varrho_M, \chi_M)| \to 0$ as $|E| \to 0$ uniformly in M and by Vitali's theorem we find $\bar{f}(\varrho_M, \chi_M) \to \bar{f}(\varrho, \chi)$ in $L^1(\Omega_{T_0})$ as $M \in \mathcal{N}$ tends to infinity. $\square$

9 Global existence of solutions to the sharp interface model

We are now in the position to state the existence result.

Theorem 2: *(Global existence for the sharp interface model with polynomial free energy)* *Let the assumptions of Section 6 hold. Then, there exists a weak solution* (ϱ, μ, χ, u) *of (6)-(12) in the sense of Section 4 such that*

(i) $\varrho \in C^{0,\frac{1}{4}}([0, T_0];\, L^2(\Omega; \mathbb{R}^n))$,
(ii) $\partial_t \varrho \in L^2(0, T_0;\, (H_0^1(\Omega; \mathbb{R}^n))')$,
(iii) $\chi \in L^\infty(0, T_0;\, BV(\Omega))$ *with* $\chi(1-\chi) = 0$ *almost everywhere in* Ω,
(iv) $u \in L^2(0, T_0;\, H^1(\Omega))$.

Remark: In general, the global solution (ϱ, μ, χ, u) in Theorem 2 will not be unique because the minimum in χ may not be uniquely defined.

Proof: We are going to prove that (ϱ, μ, χ, u) introduced in Theorem 1 is the desired weak solution in the sense of Section 4. From Equation (31) we learn

$$-\int_{\Omega_{T_0}} \partial_t \xi (\overline{\varrho}_M - \varrho_0) + \int_{\Omega_{T_0}} L \nabla \mu_M : \nabla \xi = 0$$

for all $\xi \in L^2(0, T_0;\, Y)$ with $\partial_t \xi \in L^2(\Omega_{T_0})$ and $\xi(T_0) = 0$. Passing to the limit $M \to \infty$ together with Theorem 1 this implies (14). Now we show (15). From (24) we see

$$\int_\Omega \partial_\varrho f(\varrho_M, \chi_M) \cdot \eta = \int_\Omega \mu_M \cdot \eta \quad \text{for all } \eta \in Y \cap L^\infty(\Omega; \mathbb{R}^n).$$

The convergence of

$$\int_\Omega \partial_\varrho f(\varrho_M, \chi_M) \cdot \eta \to \int_\Omega \partial_\varrho f(\varrho, \chi) \cdot \eta$$

is evident by Vitali's theorem similar to the proof of Theorem 1 by using the almost everywhere convergence of ϱ_M and χ_M, the growth condition (A2.3), Estimate (28) on $\bar{f}$ and the boundedness of η. The dominated convergence theorem of Lebesgue, the strong convergence of ϱ_M and ∇u_M in L^2 and the growth condition (A5.3) guarantee that we can perform the limit

$$\lim_{M \to \infty} \int_\Omega \partial_\varepsilon W^{el}(\varrho_M, \mathcal{E}(u_M)) \cdot \zeta.$$

Similarly, we can pass to the limit in Equation (25). $\square$

10 Logarithmic free energy

In the following 3 sections we are going to extend Theorem 2 to logarithmic free energies. The results will be valid for the particular free energy functional that is most interesting to us,

$$f(\varrho, \chi, u) = \chi\alpha_1 \sum_{j=1}^{n} \varrho_j \ln \varrho_j + (1-\chi)\alpha_2 \sum_{j} \varrho_j \ln \varrho_j + W^{\mathrm{el}}(\varrho, \mathcal{E}(u)) \tag{32}$$

and we will exploit the particular structure of f in the following.

As is well known the mathematical discussion is much more subtle, f becomes singular as one ϱ_j approaches 0. To show that $0 < \varrho_j < 1$ for every j, we approximate f for $\delta > 0$ by some f^δ that fulfils the requirements of Section 6 and find suitable a-priori estimates that allow to pass to the limit $\delta \to 0$.

Despite of the mathematical difficulties, the logarithmic free energy guarantees that the concentration vector ϱ lies in the transformed Gibbs simplex

$$G := \Sigma \cap \{\varrho \in \mathbb{R}^n \mid \varrho_j \geq 0 \text{ for } 1 \leq j \leq n\}$$

and is therefore physically meaningful.

The assumptions (A2) and (A3) of Section 6 are replaced by the following ones:

(A2') f is of the form (32) with $\alpha_1 > 0$, $\alpha_2 > 0$.

(A3') The initial value $\varrho_0 = (\varrho_{01}, \ldots, \varrho_{0n}) \in X_1$ fulfils $\varrho_0 \in G$ almost everywhere and

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

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 [10] by Elliott and Luckhaus.

Due to Assumption (A2') this leads to

$$f^\delta = \bar{f}^\delta + W^{\mathrm{el}}(\mathcal{E}(u)), \tag{33}$$

$$\bar{f}^\delta(\varrho, \chi) := \chi\alpha_1 \sum_{j=1}^{n} \psi^\delta(\varrho_j) + (1-\chi)\alpha_2 \sum_{j=1}^{n} \psi^\delta(\varrho_j). \tag{34}$$

As can be easily checked, $\bar{f}^\delta$ fulfils the assumptions of Section 6.

11 Uniform estimates

The following lemma was first stated and proved in [10] 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 (33), (34).

Lemma 4: *(Uniform bound from below on f^δ)*
There exists a $\delta_0 > 0$ and a $K > 0$ such that for all $\delta \in (0, \delta_0)$

$$f^\delta(\varrho, \chi, u) \geq -K \quad \textit{for all } \varrho \in \Sigma,\ \chi \in [0,1],\ u \in \mathbb{R}^D.$$

Now we summarise the results for the regularised problem proved in Lemma 3 and Theorem 1. Lemma 5 also states the boundedness and convergence of the numerical solutions as $\delta \searrow 0$.

Lemma 5: *(A-priori and compactness results for the regularised problem)*
(a) For all $\delta \in (0, \delta_0)$ there exists a weak solution $(\varrho^\delta, \mu^\delta, \chi^\delta)$ of (6)-(12) with a logarithmic free energy that satisfies (A2'), (A3'), (A4)-(A6) in the sense of Section 4.
(b) There exists a constant $C > 0$ independent of δ such that for all $\delta \in (0, \delta_0)$

$$\begin{aligned} \sup_{t\in[0,T_0]} \left\{ \|\varrho^\delta(t)\|_{L^2} + \|\chi^\delta(t)\|_{BV} + \|u^\delta(t)\|_{H^1} \right\} &\leq C, \\ \sup_{t\in[0,T_0]} \int_\Omega \bar{f}^\delta(\varrho^\delta(t), \chi^\delta(t)) + \|\nabla\mu^\delta\|_{L^2(\Omega_{T_0})} &\leq C \end{aligned}$$

and

$$\|\varrho^\delta(t_2) - \varrho^\delta(t_1)\|_{L^2} \leq C|t_2 - t_1|^{\frac{1}{4}}$$

for all $t_1, t_2 \in [0, T_0]$.
(c) One can extract a subsequence $(\varrho^\delta)_{\delta\in\mathcal{R}}$, where $\mathcal{R} \subset (0, \delta_0)$ is a countable set with zero as the only accumulation point such that

$$\begin{array}{lll}
(i) & \varrho^\delta & \to \varrho \textit{ in } C^{0,\alpha}([0,T_0];\ L^2(\Omega;\mathbb{R}^n)) \textit{ for all } \alpha \in (0, \tfrac{1}{4}), \\
(ii) & \varrho^\delta & \to \varrho \textit{ in } L^\infty(0,T_0;\ L^2(\Omega;\mathbb{R}^n)), \\
(iii) & \varrho^\delta & \to \varrho \textit{ almost everywhere in } \Omega_{T_0}, \\
(iv) & \varrho^\delta & \overset{*}{\rightharpoonup} \varrho \textit{ in } L^\infty(0,T_0;\ L^2(\Omega;\mathbb{R}^n)), \\
(v) & \mu^\delta & \rightharpoonup \mu \textit{ in } L^2(0,T_0;\ H^1_0(\Omega;\mathbb{R}^n)), \\
(vi) & u^\delta & \to u \textit{ in } L^2(0,T_0;\ H^1(\Omega)), \\
(vii) & \chi^\delta & \to \chi \textit{ almost everywhere in } \Omega_{T_0}, \\
(viii) & \chi^\delta & \to \chi \textit{ in } L^\infty(0,T_0;\ BV(\Omega)) \textit{ with } \chi(1-\chi) = 0 \textit{ a.e. in } \Omega, \\
(ix) & \partial_\varrho \bar{f}(\varrho^\delta, \chi^\delta) & \to \partial_\varrho \bar{f}(\varrho, \chi) \textit{ in } L^1(\Omega_{T_0})
\end{array}$$

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

Proof: Using Lemma 4, the regularised problem satisfies the assumptions of Section 6 and by Theorem 2, a weak solution for fixed $\delta \in (0, \delta_0)$ exists. This proves (a). Lemma 3 and Theorem 1 imply directly (b). From Lemma 3 it follows that $F^\delta(\varrho_0, \chi_0, u_0)$ does not depend on δ, hence the constant on the right hand side does not depend on δ.
Theorem 1 leads to Assertion (c). □

12 Global existence of solutions for logarithmic free energies

Theorem 3: *(Global existence for the sharp interface model with logarithmic free energy)* *Let the assumptions of Section 10 hold. Then, there exists a weak solution (ϱ, μ, χ, u) in the sense of Section 4 of the sharp interface equations (6)-(12) with logarithmic free energy such that*

(i) $\varrho \in C^{0,\frac{1}{4}}([0,T_0];\, L^2(\Omega;\mathbb{R}^n))$,
(ii) $\partial_t\varrho \in L^2(0,T_0;\, (H^1_0(\Omega;\mathbb{R}^n))')$,
(iii) $\chi \in L^\infty(0,T_0;\, BV(\Omega))$,
(iv) $u \in L^\infty(0,T_0;\, H^1(\Omega,\mathbb{R}^D))$,
(v) $\ln\varrho_j \in L^1(\Omega_{T_0})$ *for* $1 \le j \le n$ *and in particular* $0 < \varrho_j < 1$ *almost everywhere.*

Proof: We pass to the limit $\delta \searrow 0$ in the weak formulation (14)-(17) with f defined by (32) and have to show that (ϱ, μ, χ, u) found in Lemma 5 is a solution. The limit for (14) and (16) can be justified in the same way as in the proof of Theorem 2. It remains to control the limit $\delta \searrow 0$ in (15). We have

$$\chi^\delta\alpha_1\sum_{k=1}^n \varphi^\delta(\varrho_k^\delta) + (1-\chi^\delta)\alpha_2\sum_{k=1}^n \varphi^\delta(\varrho_k^\delta) = \mu^\delta - \partial_\varrho W^{\mathrm{el}}(\varrho^\delta, \mathcal{E}(u^\delta)).$$

As $\nabla u^\delta \in L^2(\Omega_{T_0})$, we have $\partial_\varrho W^{el}(\varrho^\delta, \mathcal{E}(u^\delta)) \in L^2(0,T_0;\; L^1(\Omega))$ and from Lemma 5 $\mu^\delta \in L^2(0,T_0;\; H^{1,2}(\Omega))$. Since additionally $\alpha_1 > 0$, $\alpha_2 > 0$ and $\mu^\delta(1-\mu^\delta) \equiv 0$ in Ω_{T_0}, we find

$$\|\varphi^\delta(\varrho_k^\delta)\|_{L^1(\Omega_{T_0})} \le C. \tag{35}$$

Now we will show that $\varphi^\delta(\varrho_k^\delta)$ converges to $\varphi(\varrho_k)$ almost everywhere in Ω_{T_0}. From the almost everywhere convergence of ϱ_k^δ to ϱ_k, (35) and the Lemma of Fatou we find

$$\int\limits_{\Omega_{T_0}} \liminf_{\delta\searrow 0} |\varphi^\delta(\varrho_k^\delta)| \le \liminf_{\delta\searrow 0} \int\limits_{\Omega_{T_0}} |\varphi^\delta(\varrho_k^\delta)| \le C.$$

Next we will show that

$$\lim_{\delta\searrow 0}\varphi^\delta(\varrho_k^\delta) = \begin{cases} \varphi(\varrho_k) & \text{if } \lim_{\delta\searrow 0}\varrho_k^\delta = \varrho_k \in (0,1), \\ \infty & \text{if } \lim_{\delta\searrow 0}\varrho_k^\delta = \varrho_k \notin (0,1) \end{cases} \tag{36}$$

almost everywhere in Ω_{T_0}. For a point $(x,t) \in \Omega_{T_0}$ with $\lim_{\delta\searrow 0}\varrho_k^\delta(x,t) = \varrho_k(x,t)$, we obtain from $\varphi^\delta(d) = \varphi(d)$ for $d \ge \delta$ that $\varphi^\delta(\varrho^\delta(x,t)) \to \varphi(\varrho(x,t))$ as $\delta \searrow 0$. In the second case of a point $(x,t) \in \Omega_{T_0}$ with $\lim_{\delta\searrow 0}\varrho_k^\delta(x,t) = \varrho_k(x,t) \le 0$, we have for δ small enough

$$|\varphi^\delta(\varrho_k^\delta(x,t))| \ge \varphi(\max\{\delta, \varrho_k^\delta(x,t)\}) \to \infty \quad \text{for } \delta \searrow 0.$$

This proves (36).

From (36) and (35) we deduce $0 < \varrho_k < 1$ almost everywhere, $\int\limits_{\Omega_{T_0}} |\varphi(\varrho_k)| \le C$ and $\varphi^\delta(\varrho_k^\delta) \to \varphi(\varrho_k)$ almost everywhere. With Vitali's theorem we find

$$\varphi^\delta(\varrho_k^\delta) \to \varphi(\varrho_k) \quad \text{in } L^1(\Omega_{T_0}).$$

Since $\chi^\delta \to \chi$ almost everywhere in Ω_{T_0}, we can pass to the limit in (15). $\square$

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