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Existence and Uniqueness for a Model Describing Chalcopyrite Disease Within Sphalerite

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ABSTRACT

We show global existence and uniqueness for a system of partial differential equations that is a model for chalcopyrite disease within sphalerite. Using direct methods in the calculus of variations, we proof existence of a solution to an implicit time discretisation, derive uniform bounds and pass to the limit. By considering a regularised problem, it is possible to extend the existence results to logarithmic free energies. Furthermore, by an integration in time method we can show uniqueness of the solution. Additionally a free energy inequality affirms thermodynamical correctness of the model.

Key Words: Phase transitions; Reaction diffusion equations; Galerkin approximation.

1. INTRODUCTION

This article is devoted to the mathematical analysis of a certain system of partial differential equations that models the so-called chalcopyrite disease within

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sphalerite. The formulation consists of reaction diffusion equations combined with a modified Allen–Cahn equation.

The particular aspect about chalcopyrite disease is that the segregation process depends upon a diffusor, here copper, that penetrates the crystal from outside and causes an oxidation of the mineral. In those regions of the crystal that are copper rich the chalcopyrite phase is energetically more favorable, which is the reason for the observed concentration of chalcopyrite phases within sphalerite close to the domain boundaries after the segregation process. The general class of phenomena that show this peculiarity has been called *diffusion induced segregation processes*.

In Blesgen et al. (2002) a derivation of the mathematical model is found. This work also explains the physical background, gives references on the mineralogical experiments, and provides some numerical computations.

The objective of the present work is to complete the justification of the model and proof global existence and uniqueness of the solution. The article is organised in the following way. We start with a restatement of the equations, add some necessary notations and state the function spaces. Next a free energy inequality is derived that shows the thermodynamical correctness of the model in the isothermal setting. The proof of existence is then done in two steps. The first part, found in Secs. 4–9, discusses the case of polynomial free energies. The growth conditions in Sec. 6 are set up accordingly.

The second step, carried out in Secs. 10–13, generalises to logarithmic free energies. For the proof, a regularised functional is introduced leading to a regularised problem to which the results for the polynomial free energy are applied. The last Sec. 14 is devoted to a uniqueness result.

Similar problems have been considered for the Cahn–Hilliard system, the Allen–Cahn equation and other related equations, see in particular the works of Garcke (2001), Elliott and Luckhaus (1991), Blowey and Elliott (1991) and Barrett and Blowey (1995). The techniques employed here are also related to the earlier work (Alt and Luckhaus, 1983). The principle of showing compactness results for a discrete model that allow to pass to the limit of a continuum model is classical and goes back to the work of Leray (1934).

The main difficulty of the system analysed here lies in the presence of a reaction term that has severe implications on the variational structure of the problem.

2. PRELIMINARIES

Let us first restate the mathematical model. Let Ω be a bounded domain in $\mathbb{R}^n$ with Lipschitz boundary and $\Omega_D := \Omega \times (0, D)$ for chosen $D > 0$. With $c = (c_1, \dots, c_4)$ we denote the concentration vector related to the chemical substances

$$c_1 \approx Fe^{3+}, \quad c_2 \approx Fe^{2+}, \quad c_3 \approx Cu^{+}, \quad c_4 \approx Zn^{2+}, \quad c_5 \approx \text{vacancies}.$$

As $c_5 = (1/2)c_1$, see Blesgen et al. (2002), the solution vector c has 4 components. The corresponding chemical potentials are denoted by μ_j and $\chi \in (0, 1)$ is a phase parameter, where e.g., $\chi(x, t) = 0$ means that in $(x, t) \in \Omega_D$ the sphalerite phase is present and $\chi(x,t) = 1/2$ means that the system is in (x,t) in an intermediate state with no dominant phase.

We are concerned with the problem

Find for $t \geq 0$ the vector (c, μ, χ) with $c = (c_1, c_2, c_3, c_4)$ such that in Ω_D

$$\partial_t c = \operatorname{div}(L\nabla\mu) + r(c), \tag{1}$$

$$\mu = \frac{\partial f}{\partial c} - \operatorname{div}(\Lambda\nabla c), \tag{2}$$

$$\tau\partial_t\chi = \gamma\triangle\chi - \psi(c_3, \chi) \tag{3}$$

and for $t = 0$ in Ω

$$c(\cdot, 0) = c_0(\cdot), \quad \chi(\cdot, 0) = \chi_0(\cdot) \tag{4}$$

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

$$c_i = \mu_i = 0, \quad 1 \leq i \leq 4. \tag{5}$$

In (1)–(5), L is a positive definite matrix, $\Lambda : \mathbb{R}^{4\times n} \to \mathbb{R}^{4\times n}$ a positive definite tensor, $\tau > 0$ a scaling constant, $\gamma > 0$ is the square of the interface thickness, $\psi = \partial_\chi f$, and the reaction term for the reformulated problem is (for constants $k,\ \kappa > 0$)

$$r(c) = (k(c_2 - \kappa c_1 c_3), -k(c_2 - \kappa c_1 c_3), 0, 0).$$

The free energy density without surface energy terms is defined by

$$f = f(c, \chi) = \chi f_1(c) + (1-\chi) f_2(c), \tag{6}$$

$$f_k = \sum_{j=1}^{5} \beta_j^k c_j \ln c_j + \left(\sum_{j=1}^{5} \alpha_j c_j\right)^2, \quad k = 1, 2 \tag{7}$$

with densities f_1 for chalcopyrite and f_2 for sphalerite. $W \geq 0$ is a double well potential and $\alpha_j, \beta_j^k \geq 0$. The logarithmic shape of f in (7) has its origin in random pairwise interactions (order-disorder phase transition) and can be derived from statistical mechanics. The complete free energy F with surface energy terms is defined in (27) below.

As $(1/2)c_1$ yields the concentration of the lattice vacancies, the concentration vector c lies in the simplex

$$c \in \Sigma := \left\{ d = (d_1, \ldots, d_4) \in \mathbb{R}^4 \;\middle|\; \frac{3}{2}d_1 + d_2 + d_3 + d_4 = 1 \right\}.$$

We do not propose $0 \leq c_i \leq 1$ in Ω because for the polynomial free energies treated in the first part this is simply not true. This is one of the reasons to introduce logarithmic free energies. Let

$$X_1 := \{ c \in H_0^{1,2}(\Omega; \mathbb{R}^4) \parallel c \in \Sigma \text{ almost everywhere} \},$$

$$X_2 := H^{1,2}(\Omega; \mathbb{R}),$$

where $H^{m,2}(\Omega)$ denotes the space of m-times weakly differentiable functions in the Hilbert space $L^2(\Omega)$ and $H_0^{m,2}(\Omega)$ is the closure of $C_0^\infty(\Omega)$ w.r.t. to $\|\cdot\|_{H^{1,2}}$.

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

$$Y := H_0^{1,2}(\Omega; \mathbb{R}^4)$$

and its dual

$$\mathscr{D} := (H_0^{1,2}(\Omega; \mathbb{R}^4))' = H^{-1,2}(\Omega; \mathbb{R}^4).$$

Let us now regard the mapping $\mathscr{L}(w) : Y \to \mathscr{D}$ corresponding to $w \mapsto -\mathrm{div}(L\nabla w)$ with Dirichlet boundary conditions, given by

$$\mathscr{L}(w)(\zeta) := \int_\Omega L\nabla w : \nabla\zeta.$$

The existence of $\mathscr{G}$ is derived from the Poincaré inequality and the Lax–Milgram theorem, since L is positive definite. From this we find that $\mathscr{G}$ is positive definite, self-adjoint, injective and compact.

Hence we have

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

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

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

with the corresponding norm

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

Functions $v \in Y$ canonically define an element in Y and consequently, $(\cdot,\cdot)_L$ and $\|\cdot\|_L$ are defined for elements in Y, too.

With the help of Young's inequality we find for $\delta > 0$ and all $d \in Y$ the estimate:

$$\begin{aligned}\|d\|_{L^2} &= (L\nabla\mathscr{G}d, \nabla d)_{L^2} \\ &\le \|L^{1/2}\nabla\mathscr{G}d\|_{L^2}\|L^{1/2}\nabla d\|_{L^2} \\ &\le \frac{C_L}{\delta}\|d\|_L^2 + \delta\|\nabla d\|_{L^2}^2, \end{aligned} \tag{8}$$

where C_L is a positive constant depending on L.

The Green's function $\mathscr{G}$ allows to rewrite the conservation of mass equations as

$$\mathscr{G}(\partial_t c - r(c)) = \mu := \left(\frac{\partial f}{\partial c_j}\right)_{1\le j\le 4} - \mathrm{div}(\Lambda\nabla c). \tag{9}$$

3. FREE ENERGY INEQUALITY

We want to derive a free energy estimate for the isothermal system. In this section we denote by f the free energy density including surface energy terms, as this is more intuitive for the calculations to come. With $J = -L\nabla\mu$ we can recast (1)–(5) as

$$\partial_t c + \operatorname{div}(J) = r, \tag{10}$$

$$\partial_c f - \operatorname{div}\frac{\partial f}{\partial \nabla c} = \mu, \tag{11}$$

$$\tau \partial_t \chi = -\partial_\chi f. \tag{12}$$

An application of the chain rule yields:

$$\frac{d}{dt} f(c, \nabla c, \chi) = \sum_{j=1}^{4} \frac{\partial f}{\partial c_j} \partial_t c_j + \sum_{j=1}^{4} \frac{\partial f}{\partial \nabla c_j} \cdot \nabla \partial_t c_j + \frac{\partial f}{\partial \chi} \partial_t \chi. \tag{13}$$

From this identity we learn that we have to test the equation for c_i with $\partial f/\partial c_i$, $1 \leq i \leq 4$ and Eq. (12) with $\partial f/\partial \chi$. Integrating over Ω and after one integration by parts we obtain:

$$\frac{d}{dt} \int_\Omega f(c, \nabla c, \chi) = \int_\Omega \left[\sum_{j=1}^{4} \left(\frac{\partial f}{\partial c_j} - \operatorname{div}\left(\frac{\partial f}{\partial \nabla c_j} \right) \right) \partial_t c_j + \frac{\partial f}{\partial \chi} \partial_t \chi \right] + \int_{\partial\Omega} \sum_{j=1}^{4} \partial_t c_j \frac{\partial f}{\partial \nabla c_j} \cdot \vec{\nu}.$$

Due to (11) this formulation is equivalent to:

$$\frac{d}{dt} \int_\Omega f(c, \nabla c, \chi) - \int_\Omega \left(\sum_{j=1}^{4} \nabla \mu_j \cdot J_j + \frac{\partial f}{\partial \chi} \partial_t \chi + \mu \cdot r \right) + \int_{\partial\Omega} \left(\sum_{j=1}^{4} \mu_j J_j - v \right) \cdot \vec{\nu} = 0. \tag{14}$$

This is the constitutive equality for the Helmholtz free energy density f.

In (14), the second term of the boundary integral

$$v := \sum_{j=1}^{4} \partial_t c_j \frac{\partial f}{\partial \nabla c_j} \tag{15}$$

is physically motivated and can be understood as an interface flux between the transition layers of the non-equilibrium phases, see Gurtin (1989) and Alt and Pawlov (1992). To recast (14) as an inequality, we notice that due to the positive definiteness of the matrix L,

$$\sum_{j=1}^{4} \nabla \mu_j \cdot J_j \leq 0. \tag{16}$$

Additionally, by (12), we have $\left(\partial f/\partial \chi\right) \partial_t \chi \leq 0$.

In order to estimate $\int_\Omega \mu \cdot r$, we have to exploit the particular form of $r = (r_1, -r_1, 0, 0)$ and f. The logarithms in the free energy guarantees $c_1 > 0$, $c_2 > 0$ in Ω for $t > 0$ if this is true for $t = 0$. In Theorem 2 a rigorous proof of this statement will be given. Let

$$\sigma_1 := \sup_{x\in\Omega} c_{01}(x), \quad \sigma_2 := \inf_{x\in\Omega} c_{02}(x)$$

where σ_1, σ_2 are positive constants. By the parabolic maximum principle, (Protter and Weinberger, 1967), we have $\sigma_1 = \sup_{\Omega_D} c_1$ and $\sigma_2 = \inf_{\Omega_D} c_2$. Then a sufficient condition for $r_1 \geq 0$ in Ω_D is

$$\kappa \leq \frac{\sigma_2}{\sigma_1}. \tag{17}$$

Now we find conditions that guarantee $\mu \cdot r = (\mu_1 - \mu_2) r_1 \leq 0$. For shortness we use the notations

$$\beta_j^\chi := \chi\beta_j^1 + (1-\chi)\beta_j^2,$$
$$Q(c) := \Big(\sum_i \alpha_i c_i\Big)^2.$$

Now we postulate

$$\alpha_1 \leq \alpha_2. \tag{18}$$

This is a condition on the ion radii of Fe^{2+} and Fe^{3+} and is fulfilled in nature. Equation (18) implies $\partial_{c_1} Q(c) - \partial_{c_2} Q(c) \leq 0$. A direct calculation reveals

$$\begin{aligned} \mu_1 - \mu_2 &= \left(\beta_1^\chi + \frac{\beta_5^\chi}{2}\right)(\ln c_1 + 1) - \beta_2^\chi(\ln c_2 + 1) - \beta_5^\chi \ln 2 + \partial_{c_1} Q(c) - \partial_{c_2} Q(c) \\ &\leq \left(\beta_1^\chi + \frac{\beta_5^\chi}{2}\right)(\ln \sigma_1 + 1) - \beta_2^\chi(\ln c_2 + 1) - \beta_5^\chi \ln 2 \end{aligned}$$

where in the last line (17) and (18) were exploited. With the abbreviations

$$B_1 := \min_{j=1,2}\left\{\beta_1^j + \frac{\beta_5^j}{2}\right\}, \quad B_2 := \max_{j=1,2}\{\beta_2^j\}, \quad B_3 := \max_{j=1,2}\{\beta_5^j\}$$

we are led to the sufficient condition

$$(B_1 - B_2)(\ln\sigma_1 + 1) - B_3 \ln 2 \leq B_2 \ln\kappa. \tag{19}$$

While (17) bounds κ from above, condition (19) bounds κ from below and is simultaneously a condition on the coefficients β_1^j, β_2^j and β_5^j.

To summarise, if the reaction rate κ fulfils the conditions (17) and (19) and if (18) holds, we obtain $\mu \cdot r \leq 0$ in Ω_D. From now on we assume without further stating that this is the case.

This allows to rewrite (14) as the *constitutive free energy inequality*

$$\frac{d}{dt}\int_{\Omega} f + \int_{\partial\Omega}\left(\sum_{j=1}^{4}\mu_j J_j - v\right)\cdot\vec{v} \le 0. \tag{20}$$

We notice that according to boundary conditions (5), the boundary fluxes $\sum_j \mu_j J_j$ and v in (20) vanish along $\partial\Omega$. A different way to guarantee that the boundary fluxes vanish in (20) is to impose the Neumann boundary condition

$$\partial_\nu c_j = \partial_\nu \chi = 0 \quad \text{on } \partial\Omega,\ \ 1 \le j \le 4$$

and instead of the Dirichlet condition for μ the natural boundary conditions

$$\partial_\nu J_i = 0 \quad \text{on } \partial\Omega,\ \ 1 \le i \le 4$$

associated to the minimum problem of the free energy integral.

4. THE WEAK FORMULATION OF THE PROBLEM

A triple $(c, \mu, \chi) \in L^2(0, T_0;\ H_0^{1,2}(\Omega; \mathbb{R}^4)) \times L^2(0, T_0;\ H_0^{1,2}(\Omega; \mathbb{R}^4)) \times L^2(0, T_0;$ $H^{1,2}(\Omega; \mathbb{R}))$ with $r(c), \psi(c, \chi) \in L^1(\Omega_D)$ is called a *weak solution of* (1)–(5) if

$$-\int_{\Omega_{T_0}} \partial_t \xi \cdot (c - c_0) + \int_{\Omega_{T_0}} L\nabla\mu : \nabla\xi - \int_{\Omega_{T_0}} r(c)\xi = 0 \tag{21}$$

for all $\xi \in L^2(0, T_0;\ H_0^1(\Omega; \mathbb{R}^4))$ with $\partial_t \xi \in L^2(\Omega_D),\ \xi(T_0) = 0$, and

$$\int_{\Omega_{T_0}} \mu \cdot \eta = \int_{\Omega_{T_0}} \left(\frac{\partial f}{\partial c}(c)\cdot\eta + \Lambda\nabla c : \nabla\eta\right) \tag{22}$$

for all $\eta \in L^2(0, T_0;\ H_0^1(\Omega; \mathbb{R}^4))$ and

$$-\int_{\Omega_{T_0}} \tau\partial_t\zeta(\chi - \chi_0) + \int_{\Omega_{T_0}} \gamma\nabla\chi\cdot\nabla\zeta - \int_{\Omega_{T_0}} \psi(c, \chi)\zeta = 0 \tag{23}$$

for all $\zeta \in L^2(0, T_0;\ H^1(\Omega; \mathbb{R}))$ with $\partial_t\zeta \in L^2(\Omega_D),\ \zeta(T_0) = 0$.

5. A SEMI-IMPLICIT TIME DISCRETISATION

We fix an $M \in \mathbb{N}$ and set $h := T_0/M$. For $m \ge 1$ and given $(c^{m-1}, \mu^{m-1}, \chi^{m-1})$, consider

$$\frac{c^m - c^{m-1}}{h} = \operatorname{div}(L\nabla\mu^m) + r(c^{m-1}), \tag{24}$$

$$\mu^m = \frac{\partial f}{\partial c}(c^m, \chi^m) - \operatorname{div}(\Lambda\nabla c^m), \tag{25}$$

$$\tau\frac{\chi^m - \chi^{m-1}}{h} = \gamma\triangle\chi^m + \psi(c^m, \chi^m). \tag{26}$$

Here, $\psi(c, \chi) = \partial_\chi f(c, \chi)$ and for the following sections, let $r^{m-1} := r(c^{m-1})$.

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Apparently, (24)–(26) is the implicit time discretisation of system (1)–(5) except for the reaction term r that has been treated explicitly. Therefore, we call the resulting scheme semi-implicit.

6. STRUCTURAL ASSUMPTIONS

In order to be able to establish the existence of weak solutions in the sense of Sec. 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 decomposed,

$$f(c,\chi) = f^1(c,\chi) + f^2(c,\chi) \quad \text{for all } c \in \mathbb{R}^4,\ \chi \in \mathbb{R}$$

with $f^1, f^2 \in C^1(\mathbb{R}^4 \times \mathbb{R}; \mathbb{R})$ and $f^1(\cdot,\chi)$ convex for every $\chi \in \mathbb{R}$, $f^1(c,\cdot)$ convex for every $c \in \mathbb{R}^4$. Furthermore,

(A2.1) $f^1 \geq 0$.
(A2.2) There exists a constant $C_1 > 0$ such that

$$|\partial_c f^2(c,\chi)| \leq C_1(|c|+1) \quad \text{for all } c \in \Sigma, \chi \in \mathbb{R},$$
$$|\partial_\chi f^2(c,\chi)| \leq C_1(|\chi|+1) \quad \text{for all } c \in \Sigma, \chi \in \mathbb{R}.$$

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

$$\begin{aligned} &|\partial_c f^1(c,\chi)| + |\partial_\chi f^1(c,\chi)| \\ &\quad \leq \delta f^1(c,\chi) + C_\delta \quad \text{for all } c \in \Sigma,\ \chi \in \mathbb{R}. \end{aligned}$$

(A3) Λ is a constant, symmetric, positive definite linear mapping of $\mathbb{R}^{4\times D} \to \mathbb{R}^{4\times D}$ and there exists a constant $\lambda_0 > 0$ such that

$$M : \Lambda M \geq \lambda_0 |M|^2 \quad \text{for all } M \in \mathbb{R}^{4\times D}.$$

(A4.1) The diffusion tensor L is assumed to be symmetric and positive definite.
(A4.2) $\gamma > 0$ is a constant.

(A5) The initial data (c_0, χ_0) fulfils

$$f(c_0,\chi_0) < \infty, \quad \psi(c_0,\chi_0) < \infty.$$

By Assumption (A2) any polynomial growth is allowed for f^1, whereas exponential growth is not. For the non-convex part, sublinear growth of $\partial_c f^2$ in c and $\partial_\chi f^2$ in χ is prescribed.

From now on we assume that the Assumptions (A1)–(A5) hold.

7. EXISTENCE OF SOLUTIONS TO THE TIME DISCRETE SCHEME

For the treatment of the diffuse interface model, it is suitable to introduce the free energy functional

$$F(c, \chi) := \int_\Omega \left(f(c, \chi) + \frac{1}{2}\nabla c : \Lambda \nabla c + \frac{\gamma}{2}|\nabla \chi|^2 \right). \tag{27}$$

Additionally, for each time step m in the semi-implicit time discretisation (24)–(26), given step size $h > 0$, and given (c^{m-1}, χ^{m-1}) we define the discrete energy functional

$$F^{m,h}(c, \chi) := F(c, \chi) + \frac{1}{2h}\|c - c^{m-1} - hr^{m-1}\|_L^2 + \frac{\tau}{2h}\|\chi - \chi^{m-1}\|_{L^2}^2.$$

Lemma 1 (Existence of a minimiser). *Let* $(c^{m-1}, \chi^{m-1}) \in X_1 \times X_2$ *be given. Then, for* $0 < h < \min\{\tau/2C_1, \lambda_0/8C_1^2 C_L\}$, *the functional* $F^{m,h}$ *possesses a minimiser in* $X_1 \times X_2$.

Proof. We will show that $F^{m,h}$ is coercive and weakly lower semicontinuous. Using Assumptions (A2.1) and (A2.2), we find

$$\begin{aligned} F^{m,h}(c, \chi) &\geq \frac{\lambda_0}{2}\|\nabla c\|_{L^2}^2 + \frac{\gamma}{2}\|\nabla \chi\|_{L^2}^2 + \frac{1}{2h}\left(\|c - c^{m-1} - hr^{m-1}\|_L^2 + \tau\|\chi - \chi^{m-1}\|_{L^2}^2\right) \\ &\quad - C_1\left(\|c\|_{L^2}^2 + \|\chi\|_{L^2}^2\right) - C \\ &\geq \left(\frac{\lambda_0}{2} - \delta C_1\right)\|\nabla c\|_{L^2}^2 + \frac{\gamma}{2}\|\nabla \chi\|_{L^2}^2 + \left(\frac{1}{2h} - \frac{C_1 C_L}{\delta}\right)\|c - c^{m-1} - hr^{m-1}\|_L^2 \\ &\quad + \left(\frac{\tau}{2h} - C_1\right)\|\chi - \chi^{m-1}\|_{L^2}^2 - C, \end{aligned}$$

where in the second estimate (8) was used and $C = C(c^{m-1}, \chi^{m-1}, r)$. Now, for $0 < h < \min\{\tau/2C_1, \lambda_0/8C_1^2 C_L\}$ by choosing $\delta = \lambda_0/4C_1$, we conclude with the help of the Poincaré inequality that $F^{m,h}$ is coercive on $X_1 \times X_2$. Let

$$d := \inf\{F^{m,h}(c, \chi) \mid c \in X_1,\ \chi \in X_2\}, \quad d < \infty.$$

If we now consider a minimising sequence $(c_l, \chi_l)_{l \in N} \subset X_1 \times X_2$ with $F^{m,h}(c_l, \chi_l) \to d$, the coercivity of $F^{m,h}$ implies the boundedness of (c_l, χ_l) uniformly in l. Passing to a subsequence if necessary, by the reflexivity of $X_1 \times X_2$ we may assume

$$(c_l, \chi_l) \rightharpoonup (c, \chi) \in X_1 \times X_2 \quad \text{for } l \to \infty$$

and by Rellich's theorem or Sobolev's embedding theorem,

$$(c_l, \chi_l) \to (c, \chi) \in L^2(\Omega, \mathbb{R}^4) \times L^2(\Omega, \mathbb{R}) \quad \text{for } l \to \infty$$

and $(c_l, \chi_l) \to (c, \chi)$ a.e. in Ω.

To verify the weak lower semicontinuity of $F^{m,h}$ in $X_1 \times X_2$ we first remark that this is true for all convex terms. For $\int_\Omega f^1(c,\chi)$ this follows from Assumption (A2) and for $\int_\Omega f^2(c,\chi)$ from (A2.2) and the dominated convergence theorem of Lebesgue. This implies

$$F^{m,h}(c,\chi) \leq \liminf_{l\to\infty} F^{m,h}(c_l,\chi_l). \qquad \square$$

Lemma 2 (Euler–Lagrange equations)**.** *The minimiser* (c^m,χ^m) *of* $F^{m,h}$ *fulfils*

$$\int_\Omega \frac{c^m - c^{m-1}}{h}\cdot\xi + \int_\Omega L\nabla\mu^m : \nabla\xi = \int_\Omega r^{m-1}\xi \quad \textit{for all } \xi\in Y, \tag{28}$$

$$\int_\Omega \Lambda\nabla c^m : \nabla\eta + \partial_c f(c^m,\chi^m)\cdot\eta = \int_\Omega \mu^m\cdot\eta \quad \textit{for all } \eta\in Y\cap L^\infty(\Omega;\mathbb{R}^4), \tag{29}$$

$$\int_\Omega \left[\tau\frac{\chi^m-\chi^{m-1}}{h} + \psi(c^m,\chi^m)\right]\zeta + \int_\Omega \gamma\nabla\chi^m\cdot\nabla\zeta = 0 \quad \textit{for all } \zeta\in H^1(\Omega). \tag{30}$$

Here, $\mu^m = \mathcal{G}\big((c^m - c^{m-1}/h) - r^{m-1}\big)$.

Proof. We choose directions $\xi\in Y\cap L^\infty(\Omega;\mathbb{R}^4)$, $\zeta\in X_2\cap L^\infty(\Omega;\mathbb{R})$ and determine the variations of $F^{m,h}(c,\chi)$ with respect to c and χ for ξ, ζ. The variation w.r.t. c is

$$\lim_{s\to 0}\big((F^{m,h}(c^m+s\xi,\chi^m) - F^{m,h}(c^m,\chi^m))s^{-1}\big). \tag{31}$$

Since f^1 is convex in c, we have

$$f^1(c^m,\chi^m) \geq f^1(c^m+s\xi,\chi^m) - s\partial_c f^1(c^m+s\xi,\chi^m)\cdot\xi.$$

This implies

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

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

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

Assumption (A2.2) and Lebesgue's dominated convergence theorem imply

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

The variation of the quadratic form $c\mapsto (1/2h)\|c^m - c^{m-1} - hr^{m-1}\|_L^2$ yields

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

Hence we obtain (28). The equality (29) follows because (c^m, χ^m) is a minimiser and thus the variation in (31) is 0.

To derive (30), we consider the variation of $F^{m,h}(c^m, \chi^m)$ w.r.t. χ. As before,

$$\lim_{s\to 0}\left(\tau s^{-1}(2h)^{-1}\left(\|\chi^m + s\zeta - \chi^{m-1}\|_{L^2}^2 - \|\chi^m - \chi^{m-1}\|_{L^2}^2\right)\right) = \left(\tau\frac{\chi^m - \chi^{m-1}}{h}, \zeta\right)_{L^2}.$$

It remains to prove

$$\lim_{s\to 0}\int_\Omega \left(f(c^m, \chi^m + s\zeta) - f(c^m, \chi^m)\right) = \int_\Omega \partial_\chi f(c^m, \chi^m)\zeta.$$

Since this limit can be justified in the same way as (31), Identity (30) follows. □

8. UNIFORM ESTIMATES

In the preceeding sections we proved the existence of a discrete solution (c^m, μ^m, χ^m) for $1 \le m \le M$ and arbitrary $M \in \mathbb{N}$. We define the piecewise constant extension (c_M, μ_M, χ_M) of $(c^m, \mu^m, \chi^m)_{1\le m\le M}$ by

$$(c_M(t), \mu_M(t), \chi_M(t)) := \left(c_M^m, \mu_M^m, \chi_M^m\right) := \left(c^m, \mu^m, \chi^m\right) \quad \text{for } t \in ((m-1)h, mh]$$

and $c_M(0) = c_0$, $\chi_M(0) = \chi_0$, $\mu_M(0)$ obtained from Eq. (29).

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

$$\left(\bar{c}_M, \bar{\mu}_M, \bar{\chi}_M\right)(t) := \beta\left(c_M^m, \mu_M^m, \chi_M^m\right) + (1-\beta)\left(c_M^{m-1}, \mu_M^{m-1}, \chi_M^{m-1}\right).$$

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*

$$F(c_M, \chi_M)(t) + \frac{1}{2}\int_{\Omega_t} L\nabla\mu_M : \nabla\mu_M \le F(c_0, \chi_0).$$

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

$$\sup_{0\le t\le T_0}\left\{\|c_M(t)\|_{H^1} + \|\chi_M(t)\|_{H^1}\right\} \le C, \tag{32}$$

$$\sup_{0\le t\le T_0}\int_\Omega f^1(c_M(t), \chi_M(t)) + \|\nabla\mu_M\|_{L^2(\Omega_{T_0})} \le C. \tag{33}$$

Proof. The idea of the proof is the same as in Garcke (2001). As (c^m, χ^m) is a minimiser of $F^{m,h}$,

$$F(c^m, \chi^m) + \frac{1}{2h}\|c^m - c^{m-1} - hr^{m-1}\|_L^2 + \frac{1}{2h}\|\chi^m - \chi^{m-1}\|_{L^2}^2 \le F(c^{m-1}, \chi^{m-1}). \tag{34}$$

A direct calculation gives

$$\frac{1}{2h}\|c^m - c^{m-1} - hr^{m-1}\|_L^2 = \frac{h}{2}(\nabla\mu^m, L\nabla\mu^m)_{L^2}. \tag{35}$$

By iterating (34), Eq. (35) yields

$$F\big(c_M^m, \chi_M^m\big) + \frac{1}{2}\int_0^{mh} \big(\nabla\mu_M^m, L\nabla\mu_M^m\big)_{L^2}\, dt \le F(c_0, \chi_0).$$

Using the assumptions and with the Poincaré inequality this proves the lemma. □

We extend c_M by the initial value c_0 of c for $t \in (-h, 0]$. Now, for the linear interpolation $\bar{c}_M$ of c_M^m, the Euler–Lagrange equation (28) can be rewritten as

$$\int_\Omega \partial_t \bar{c}_M(t)\cdot\xi + \int_\Omega L\nabla\mu_M(t) : \nabla\xi = \int_\Omega r(c_M(t-h))\cdot\xi \quad \text{for all } \xi \in Y \tag{36}$$

which holds for almost all $t \in (0, T_0)$. Together with the uniform estimates of Lemma 3, (36) allows to show compactness in time.

Lemma 4 (Compactness for c_M and μ_M). *There exists a constant $C > 0$ such that for all $t_1, t_2 \in [0, T_0]$*

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

Furthermore, there is a subsequence $(c_M)_{M\in\mathcal{N}}$ and a subsequence $(\mu_M)_{M\in\mathcal{N}}$ with $\mathcal{N} \subset \mathbb{N}$ and there are $c \in L^\infty(0, T_0;\, Y)$, $\mu \in L^2(0, T_0;\, Y)$ such that

(i) $\bar{c}_M \to c$ *in* $C^{0,\alpha}([0, T_0];\, L^2(\Omega; \mathbb{R}^4))$ *for all* $\alpha \in (0, 1/4)$,
(ii) $c_M \to c$ *in* $L^\infty(0, T_0;\, L^2(\Omega; \mathbb{R}^4))$,
(iii) $c_M \to c$ *almost everywhere in* Ω_D,
(iv) $c_M \overset{*}{\rightharpoonup} c$ *in* $L^\infty(0, T_0;\, H_0^1(\Omega; \mathbb{R}^4))$,
(v) $\mu_M \rightharpoonup \mu$ *in* $L^2(0, T_0;\, H_0^1(\Omega; \mathbb{R}^4))$

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

Proof. We test Eq. (36) with $\xi := \bar{c}_M(t_2) - \bar{c}_M(t_1)$, 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

$$\|\bar{c}_M(t_2) - \bar{c}_M(t_1)\|_{L^2}^2 + \int_{t_1}^{t_2}\int_\Omega L\nabla\mu_M(t) : \nabla(\bar{c}_M(t_2) - \bar{c}_M(t_1))dt$$
$$= \int_{t_1}^{t_2}\int_\Omega r(c_M(t-h))(\bar{c}_M(t_2) - \bar{c}_M(t_1))dt.$$

The c_M^m are uniformly bounded in Y, therefore the linear interpolants $\bar{c}_M$ are uniformly bounded in $L^\infty(0, T_0;\, Y)$. Thus we obtain

$$\|\bar{c}_M(t_2) - \bar{c}_M(t_1)\|_{L^2}^2 \le C\|\bar{c}_M\|_{L^\infty(H^1)}\int_{t_1}^{t_2}\big(\|\nabla\mu_M(t)\|_{L^2} + \|r(c_M(t-h))\|_{L^2}\big)dt$$
$$\le C\|\bar{c}_M\|_{L^\infty(H^1)}\big[(t_2 - t_1)^{1/2}\|\nabla\mu\|_{L^2(\Omega_D)} + (t_2 - t_1)\|r(c_M)\|_{L^\infty(L^2)}\big].$$

Employing the a-priori estimates (32) and (33) we have shown

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

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

The boundedness of $(\bar{c}_M)$ in $L^\infty(0, T_0;\ H_0^{1,2}(\Omega))$ and the fact that $H^1(\Omega)$ is compactly embedded in $L^2(\Omega)$ yields as a consequence of the Arzelà–Ascoli theorem statement (i).

For the proof of (ii), (iii) and (iv) we choose for $t \in [0, T_0]$ values $m \in \{1, \ldots, M\}$ and $\beta \in [0, 1]$ such that $t = (\beta m + (1-\beta)(m-1))h$. From the definition of $\bar{c}$ we get at once

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

This tends to 0 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 (32) which gives the boundedness of c_M in $L^\infty(0, T_0;\ Y)$.

For the proof of (v) we notice that due to estimate (33), the $(\nabla\mu_M)$ are uniformly bounded in $L^2(\Omega_D)$. 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. □

Lemma 5 (Compactness for χ_M)**.** *For a suitable subsequence* $\mathcal{N} \subset \mathbb{N}$, *we have*

(i) $\bar{\chi}_M \to \chi$ *in* $C^{0,\alpha}([0, T_0];\ L^2(\Omega))$ *for all* $\alpha \in (0, 1/2)$,
(ii) $\chi_M \to \chi$ *in* $L^\infty(0, T_0;\ L^2(\Omega))$,
(iii) $\chi_M \to \chi$ *almost everywhere in* Ω_D,
(iv) $\chi_M \overset{*}{\rightharpoonup} \chi$ *in* $L^\infty(0, T_0;\ H^1(\Omega))$,
(v) $\partial_c f(c_M, \chi_M) \to \partial_c f(c, \chi)$ *in* $L^1(\Omega_D)$,
(vi) $\partial_\chi f(c_M, \chi_M) \to \partial_\chi f(c, \chi)$ *in* $L^1(\Omega_D)$

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

Proof. Similarly to Eq.(36) we can reformulate Identity (30) as

$$\tau\int_\Omega \partial_t\bar{\chi}_M(t)\zeta + \int_\Omega \gamma\nabla\chi_M(t)\cdot\nabla\zeta + \int_\Omega \psi(c_M(t), \chi_M(t))\zeta = 0 \quad \text{for all } \zeta \in H^1(\Omega) \tag{37}$$

which holds for almost all $t \in [0, T_0]$.

We test (37) with $\zeta := \bar{\chi}_M(t_2) - \bar{\chi}_M(t_1)$, where $t_1, t_2 \in [0, T_0]$, $t_2 > t_1$. After integration in time from t_1 to t_2 we get

$$\tau\|\bar{\chi}_M(t_2) - \bar{\chi}_M(t_1)\|_{L^2}^2 + \int_{t_1}^{t_2}\int_\Omega \gamma\nabla\chi_M(t)\cdot\nabla(\bar{\chi}_M(t_2) - \bar{\chi}_M(t_1))dt$$
$$+ \int_{t_1}^{t_2} \psi(c_M(t), \chi_M(t))\,(\bar{\chi}_M(t_2) - \bar{\chi}_M(t_1))dt = 0.$$

From the uniform boundedness of $\bar{\chi}_M$ in $L^\infty(0, T_0; H^1(\Omega))$ and in $Ł^\infty(\Omega_D)$ we obtain:

$$\int_{t_1}^{t_2}\int_\Omega \gamma\nabla\chi_M(t)\cdot\nabla(\bar{\chi}_M(t_2)-\bar{\chi}_M(t_1))dt \le c\|\bar{\chi}_M\|_{L^\infty(H^1)}\int_{t_1}^{t_2}\|\nabla\chi_M(t)\|_{L^2}\,dt,$$

$$\int_{t_1}^{t_2}\psi(c_M(t),\chi_M(t))\,(\bar{\chi}_M(t_2)-\bar{\chi}_M(t_1))dt \le c\|\bar{\chi}_M\|_{L^\infty(\Omega_D)}\int_{t_1}^{t_2}\psi(c_M(t),\chi_M(t))dt.$$

With the continuity of ψ, these estimates imply

$$\|\bar{\chi}_M(t_2)-\bar{\chi}_M(t_1)\|_{L^2} \le C|t_2-t_1|^{\frac{1}{2}} \quad \text{for all } t_1, t_2 \in [0, T_0]$$

and exactly as in Lemma 4 this yields statements (i)–(iv).

In order to prove (v) and (vi), we first notice that by Assumption (A2), $\partial_c f$ and $\partial_\chi f$ are continuous functions. Hence, by (iii) and Lemma 4(iii),

$$\partial_c f(c_M,\chi_M) \to \partial_c f(c,\chi) \text{ almost everywhere in } \Omega_D,$$

$$\partial_\chi f(c_M,\chi_M) \to \partial_\chi f(c,\chi) \text{ almost everywhere in } \Omega_D.$$

The growth condition of Assumption (A2.3) on f^1 now yields that for arbitrary $\delta > 0$ and all measurable $E \subset \Omega$

$$\int_E |\partial_c f^1(c_M,\chi_M)| \le \delta\int_E f^1(c_M,\chi_M) + C_\delta|E| \le \delta C + C_\delta|E|.$$

Therefore, $\int_E|\partial_c f^1(c_M,\chi_M)| \to 0$ as $|E| \to 0$ uniformly in M and by Vitali's theorem, $f^1(c_M,\chi_M) \to f^1(c,\chi)$ in $L^1(\Omega_D)$ as $M \in \mathcal{N}$ tends to infinity. The same result for f^2 follows directly from (A2.2) and the dominated convergence theorem of Lebesgue.

The proof of $\partial_\chi f(c_M,\chi_M) \to \partial_\chi f(c,\chi)$ exploiting (A2.3) and (A2.2) is similar. □

9. GLOBAL EXISTENCE OF SOLUTIONS FOR POLYNOMIAL FREE ENERGY

Theorem 1 (Global existence in case of polynomial free energies). *Let the assumptions of Sec.* 6 *hold. Then, there exists a weak solution* (c, μ, χ) *of the diffuse interface equations in the sense of Sec.* 4 *such that*

(i) $c \in C^{0,1/4}([0, T_0];\ L^2(\Omega; \mathbb{R}^4))$,
(ii) $\partial_t c \in L^2(0, T_0;\ (H_0^1(\Omega; \mathbb{R}^4))')$,
(iii) $\chi \in C^{0,1/2}([0, T_0];\ L^2(\Omega))$,
(iv) $\partial_t \chi \in L^2(0, T_0;\ (H_0^1(\Omega))')$.

Proof. We are going to prove that (c, μ, χ) introduced in Lemmata 4 and 5 is the desired weak solution in the sense of (21). From Eq. (36), we learn

$$-\int_{\Omega_{T_0}}\partial_t\xi(\bar{c}_M-c_0) + \int_{\Omega_{T_0}} L\nabla\mu_M : \nabla\xi + \int_{\Omega_{T_0}} r(c_M) = 0$$

for all $\xi \in L^2(0, T_0;\; Y)$ with $\partial_t \xi \in L^2(\Omega_D)$ and $\xi(T_0) = 0$. Passing to the limit $M \to \infty$ together with Lemma 4 this implies (21). Now we show (22). From (29) we see

$$\int_\Omega \Lambda \nabla c_M : \nabla \eta + \partial_c f(c_M, \chi_M) \cdot \eta = \int_\Omega \mu_M \cdot \eta \quad \text{for all } \eta \in Y \cap L^\infty(\Omega; \mathbb{R}^4).$$

The convergence of

$$\int_\Omega \Lambda c_M : \nabla \eta \to \int_\Omega \Lambda c : \nabla \eta$$

as $M \to \infty$ is clear by linearity and the convergence

$$\int_\Omega \partial_c f(c_M, \chi_M) \cdot \eta \to \int_\Omega \partial_c f(c, \chi) \cdot \eta$$

is again evident by Vitali's theorem similar to the proof of Lemma 5 by using the almost everywhere convergence of c_M and χ_M, the growth condition (A2.3), estimate (33) on f^1 and the boundedness of η. In the same way, from (37) we obtain (23). □

10. LOGARITHMIC FREE ENERGY

In the following 4 sections we are going to extend Theorem 1 to logarithmic free energies. The results will in particular be taylor made for the free energy functional in (6) and (7), but a modification towards other expressions is of course possible. It turns out that the mathematical discussion is much more subtle, since f becomes singular as one of the c_j approaches 0.

To show that $0 < c_j < 1$ for every j, we approximate f for $\delta > 0$ by some f^δ that fulfils the requirements of Sec. 6 and find suitable a-priori estimates that put us in the position to pass to the limit $\delta \to 0$.

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

$$G := \Sigma \cap \{c \in \mathbb{R}^4 | c_j \geq 0 \text{ for } 1 \leq j \leq 4\}$$

and that $\chi \in (0, 1)$. Therefore (c, χ) is physically meaningful.

The Assumptions (A2), (A3) and (A5) of Sec. 6 are replaced by the following ones:

- (A2′) f is of the form (6) with constants $\alpha_j > 0$, $\beta_j^1 > 0$, $\beta_j^2 > 0$, $T > 0$.
- (A3′) $\Lambda = \lambda \mathrm{Id}$ for a $\lambda > 0$.
- (A5′) The initial values $c_0 \in X_1, \chi_0 \in X_2$ fulfil $c_0 \in G$, $\chi \in [0, 1]$ almost everywhere and

$$\int_\Omega c_{0k} > 0 \quad \text{for } 1 \leq k \leq 4, \qquad \int_\Omega \chi > 0, \qquad \int_\Omega (1 - \chi) > 0.$$

The assumptions (A1) and (A4) are unchanged and continue to hold.

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

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

that was first introduced in Elliott and Luckhaus (1991).

The regularised free energy functional is defined in such a way that $\psi^\delta \in C^2$ and the derivative $(\psi^\delta)'$ is monotone increasing. Since the convex combination

$$\bar{f}(c, \chi) := \chi f_1(c) + (1 - \chi) f_2(c)$$

would define a non-convex functional in c if $\chi \notin [0, 1]$, we consider the following penalisation ($f^\delta = f^{1,\delta} + f^2$, see Assumption A2)

$$f^{1,\delta}(c, \chi) := \begin{cases} \chi \sum_j \beta_j^1 \psi^\delta(c_j) + (1 - \chi) \sum_j \beta_j^2 \psi^\delta(c_j) + T\,[\psi^\delta(\chi) + \psi^\delta(1 - \chi)], \\ \quad \chi \in (0, 1), \\ +\infty, \quad \text{else} \end{cases}$$

$$f^2(c, \chi) := \left(\sum_{j=1}^4 \alpha_j c_j \right)^2.$$

Since the expression $\psi^\delta(\chi) + \psi^\delta(1 - \chi)$ in the definition of f^δ implies $0 < \chi < 1$, see the proof of Lemma 8, this approximation is no mayor restriction.

As can be easily checked, the functional $F^{m,h}$ still has a minimiser (c^m, χ^m) for every m and sufficiently small h and by construction $\chi^m \in (0, 1)$. But for $\chi \in (0, 1)$, $f^{1,\delta}$ is still continuously differentiable. Since $f^{1,\delta}$, f^2 fulfil the assumptions of Sec. 6 the earlier existence results can be carried over.

11. UNIFORM ESTIMATES

Lemma 6 (Uniform bound from below on f^δ)**.** *For $\delta_0 = 1/e$ there exists a $K > 0$ such that for all $\delta \in (0, \delta_0)$*

$$f^\delta(c, \chi) \geq -K \quad \text{for all } c \in \Sigma, \ \ \chi \in [0, 1].$$

Proof. For $\delta_0 < 1/e$ one has $\psi^\delta(d) \geq -1/e$ for $\delta < \delta_0$. As β_j^k, $T > 0$, the claim follows. □

The above lemma was first stated and proved in Elliott and Luckhaus (1991). The next lemma summarises the results for the regularised problem proved in Sec. 9.

Lemma 7 (A-priori and compactness results for the regularised problem)**.**

(a) *For all $\delta \in (0, \delta_0)$ there exists a weak solution $(c^\delta, \mu^\delta, \chi^\delta)$ of* (1)–(5) *with a logarithmic free energy that satisfies* (A2′)–(A5′) *in the sense of Sec.* 4.

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

$$\sup_{t\in[0,T_0]} \left\{ \|c^\delta(t)\|_{H^1} + \|\chi^\delta(t)\|_{H^1} \right\} \le C,$$

$$\sup_{t\in[0,T_0]} \int_\Omega f^{1,\delta}(c^\delta(t), \chi^\delta(t)) + \|\nabla\mu^\delta\|_{L^2(\Omega_D)} \le C$$

and

$$\|c^\delta(t_2) - c^\delta(t_1)\|_{L^2} \le C|t_2 - t_1|^{1/4},$$
$$\|\chi^\delta(t_2) - \chi^\delta(t_1)\|_{L^2} \le C|t_2 - t_1|^{1/2}$$

for all $t_1, t_2 \in [0, T_0]$.

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

(i) $c^\delta \to c$ *in* $C^{0,\alpha}([0, T_0];\ L^2(\Omega; \mathbb{R}^4))$ *for all* $\alpha \in (0, 1/4)$,
(ii) $c^\delta \to c$ *almost everywhere in* Ω_D,
(iii) $c^\delta \overset{*}{\rightharpoonup} c$ *in* $L^\infty(0, T_0;\ H^1_0(\Omega; \mathbb{R}^4))$,
(iv) $\chi^\delta \to \chi$ *in* $C^{0,\alpha}([0, T_0];\ L^2(\Omega))$ *for all* $\alpha \in (0, 1/2)$,
(v) $\chi^\delta \to \chi$ *almost everywhere in* Ω_D *and* $0 \le \chi^\delta,\ \chi \le 1$ *almost everywhere in* Ω_D,
(vi) $\chi^\delta \overset{*}{\rightharpoonup} \chi$ *in* $L^\infty(0, T_0;\ H^1(\Omega))$,
(vii) $\mu^\delta \rightharpoonup \mu$ *in* $L^2(0, T_0;\ H^1_0(\Omega; \mathbb{R}^4))$

as $\delta \in \mathcal{R}$ tends to 0.

Proof. Using Lemma 6, the regularised problem satisfies the assumptions of Sec. 6 and by Theorem 1, a weak solution for fixed $\delta \in (0, \delta_0)$ exists. This proves (a). The estimates in (b) are a direct consequence of Lemma 3 and Lemma 4. From Lemma 3 it follows that $F^\delta(c_0, \chi_0)$ does not depend on δ, hence the constant on the right hand side is independent of δ. (c) is proved by Lemma 4 and Lemma 5. □

12. HIGHER INTEGRABILITY FOR LOGARITHMIC FREE ENERGIES

Since $\varphi^\delta := (\psi^\delta)'$ will be singular as $\delta \to 0$ 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 $0 < r < 1$, φ_r^δ is not differentiable at the zero point of φ^δ. To overcome this difficulty, for $\rho > 0$ introduce the function $\varphi_r^{\delta,\rho}$ with $\varphi_r^{\delta,\rho} = \varphi_r^\delta$ in $\mathbb{R}\backslash[0, 1]$ and define $\varphi_r^{\delta,\rho}$ in $[0, 1]$ such that $\varphi_r^{\delta,\rho}$ is a C^1 function, monotone increasing and $\varphi_r^{\delta,\rho} \to \varphi_r^\delta$ in $C^0(\mathbb{R})$ as $\rho \searrow 0$.

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For the approximation of $\varphi^\delta(\chi^\delta)$ in the modified Allen–Cahn equation it is appropriate to introduce the Dirac sequence

$$\varphi^{\delta,\varepsilon}(x) := (\varphi^\delta * J_\varepsilon)(x) := \varepsilon^{-D} \int_{\mathbb{R}^D} \varphi^\delta(x) J\left(\frac{x-y}{\varepsilon}\right) dy$$

where the kernel $J \in C^\infty(B^1(0))$ is a positive smooth polynomial (see Assumption A2). As is well known, $\varphi^{\delta,\varepsilon} \in C^\infty$ and $\varphi^{\delta,\varepsilon} \to \varphi^\delta$ in $L^p(\Omega)$ as $\varepsilon \searrow 0$ for any $p \geq 1$, see for instance Yoshida (1995).

Even though by construction $0 < \chi^\delta < 1$ almost everywhere, it might still happen that for the limit the sets $\{x \in \Omega \mid \chi = 0\}$ and $\{x \in \Omega \mid \chi = 1\}$ 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.

Lemma 8 (Integrability of the regularised free energy). *There exists a constant $C > 0$ such that for all $\delta \in (0, \delta_0)$*

(i) $\|\varphi^\delta(c_k^\delta)\|_{L^q(\Omega_D)} \leq C$ *for a* $q > 1$ *and all* $1 \leq k \leq 4$,

(ii) $\|\varphi^\delta(\chi^\delta) + \varphi^\delta(1-\chi^\delta)\|_{L^2(\Omega_D)} \leq C$.

Proof. The weak formulation (22) for the generalised chemical potential reads

$$\int_{\Omega_{T_0}} \mu^\delta \cdot \eta = \int_{\Omega_{T_0}} \left\{ \lambda \sum_{k=1}^{4} \nabla c_k^\delta \cdot \nabla \eta_k + 2\left(\alpha_k \sum_{j=1}^{4} \alpha_j c_j^\delta \right)_{1\leq k\leq 4} \cdot \eta \right\} + \int_{\Omega_{T_0}} \left[(\chi^\delta \beta_k^1 + (1-\chi^\delta)\beta_k^2) \varphi^\delta(c_k^\delta) \right]_{1\leq k\leq 4} \cdot \eta \tag{38}$$

for all $\eta \in L^2(0, T_0;\ H^1(\Omega; \mathbb{R}^4)) \cap L^\infty(\Omega_D, \mathbb{R}^4)$. In (38) we choose $\eta := (\varphi_r^{\delta,\rho}(c_k^\delta))_{1\leq k\leq 4}$ which is an admissible test function by the Sobolev embedding theorem and because $\varphi_r^{\delta,\rho} \in C^1$. We obtain

$$\int_{\Omega_{T_0}} \sum_{k=1}^{4} \mu_k^\delta \varphi_r^{\delta,\rho}(c_k^\delta) = \int_{\Omega_{T_0}} \lambda \sum_{k=1}^{4} \nabla c_k^\delta \cdot \nabla \varphi_r^{\delta,\rho}(c_k^\delta) + 2 \int_{\Omega_{T_0}} \sum_{k=1}^{4} \alpha_k \varphi_r^{\delta,\rho}(c_k^\delta) \left(\sum_{j=1}^{4} \alpha_j c_j^\delta \right) + \int_{\Omega_{T_0}} \sum_{k=1}^{4} (\chi^\delta \beta_k^1 + (1-\chi^\delta)\beta_k^2) \varphi^\delta(c_k^\delta) \varphi_r^{\delta,\rho}(c_k^\delta).$$

Due to $(\varphi_r^{\delta,\rho})' \geq 0$ and Assumption (A3$'$) we find

$$\int_{\Omega_{T_0}} \lambda \sum_{k=1}^{4} \nabla c_k^\delta \cdot \nabla \varphi_r^{\delta,\rho}(c_k^\delta) \geq 0.$$

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This implies

$$\begin{aligned}&\int_{\Omega_{T_0}} \sum_{k=1}^{4}(\chi^\delta \beta_k^1 + (1-\chi^\delta)\beta_k^2)\varphi^\delta(c_k^\delta)\varphi_r^{\delta,\rho}(c_k^\delta)\\ &\quad\le \int_{\Omega_{T_0}} \sum_{k=1}^{4}\mu_k^\delta \varphi_r^{\delta,\rho}(c_k^\delta) - 2\int_{\Omega_{T_0}} \sum_{k=1}^{4}\alpha_k \varphi_r^{\delta,\rho}(c_k^\delta)\left(\sum_{j=1}^{4}\alpha_j c_j\right)\\ &\quad\le C(\alpha)\max_{1\le k\le 4}\|\varphi_r^{\delta,\rho}(c_k^\delta)\|_{L^2(\Omega_{T_0})}\left(\|\mu^\delta\|_{L^2(\Omega_{T_0})} + \|c^\delta\|_{L^2(\Omega_{T_0})}\right).\end{aligned}$$

For $\rho \searrow 0$ employing Lemma 6 and Lemma 7 this proves

$$\int_{\Omega_{T_0}} \sum_{k=1}^{4}(\chi^\delta \beta_k^1 + (1-\chi^\delta)\beta_k^2)\varphi^\delta(c_k^\delta)\varphi_r^\delta(c_k^\delta) \le C. \tag{39}$$

A direct computation finally yields

$$\begin{aligned}\int_{\Omega_{T_0}} \sum_{k=1}^{4}(\chi^\delta \beta_k^1 + (1-\chi^\delta)\beta_k^2)\varphi^\delta(c_k^\delta)\varphi_r^\delta(c_k^\delta) &\ge \int_{\Omega_{T_0}} \max_{1\le k\le 4}(\chi^\delta \beta_k^1 + (1-\chi^\delta)\beta_k^2)|\varphi^\delta(c_k^\delta)|^{r+1}\\ &\ge \int_{\Omega_{T_0}} C\max_{1\le k\le 4}|\varphi^\delta(c_k^\delta)|^{r+1}\end{aligned}$$

for a constant $C = C(\beta^1, \beta^2)$. The last estimate is possible because $\chi^\delta \beta_k^1 + (1-\chi^\delta)\beta_k^2 > 0$ almost everywhere in Ω_D. Together with (39) this proves (i).

Next we consider the weak formulation (23)

$$\begin{aligned}&-\int_{\Omega_{T_0}} \tau\partial_t\zeta(\chi^\delta - \chi_0) + \int_{\Omega_{T_0}} \gamma\nabla\chi^\delta\cdot\nabla\zeta - \int_{\Omega_{T_0}}\left(\sum_{j=1}^{4}\beta_j^2\psi^\delta(c_j^\delta) - \sum_{j=1}^{4}\beta_j^1\psi^\delta(c_j^\delta)\right)\zeta\\ &\quad + \int_{\Omega_{T_0}} T(\varphi^\delta(\chi^\delta) + \varphi^\delta(1-\chi^\delta))\zeta = 0\end{aligned} \tag{40}$$

of the Allen–Cahn equation. We want to test Eq. (40) with $\zeta := \varphi^{\delta,\varepsilon}(\chi) + \varphi^{\delta,\varepsilon}(1-\chi)$. Since by Theorem 1, $\chi^\delta \in C^{0,1/2}(0, T_0; L^2(\Omega_D))$, we can use Fourier theory to formally shift a half time derivative from ζ to $\chi^\delta - \chi_0$. After this procedure we find with Lemma 7

$$\int_{\Omega_{T_0}} \tau\partial_t{}^{1/2}(\varphi^{\delta,\varepsilon}(\chi^\delta) + \varphi^{\delta,\varepsilon}(1-\chi^\delta))\partial_t{}^{1/2}(\chi^\delta - \chi_0) \le C.$$

To estimate the second integral in (40) we notice

$$\int_{\Omega_{T_0}} \gamma\nabla\chi^\delta\cdot\nabla(\varphi^{\delta,\varepsilon}(\chi^\delta) + \varphi^{\delta,\varepsilon}(1-\chi^\delta)) = \int_{\Omega_{T_0}} \gamma|\nabla\chi^\delta|^2\,[(\varphi^{\delta,\varepsilon})'(\chi^\delta) - (\varphi^{\delta,\varepsilon})'(1-\chi^\delta)].$$

By Lemma 7, χ^δ is bounded in $L^\infty(0, T_0; H^1(\Omega))$ which implies the boundedness of the integral.

If we choose δ sufficiently small in (i) we find $c_j \in (0,1)$ for $1 \le j \le 4$, see also the proof of Theorem 2 below. This guarantees that $\psi^\delta(c_j)$ does not become singular and thus proves the boundedness of the third integral in (40) independently of δ. Finally we have

$$0 \le \int_{\Omega_{T_0}} (\varphi^\delta(\chi^\delta) + \varphi^\delta(1-\chi^\delta))(\varphi^{\delta,\varepsilon}(\chi^\delta) + \varphi^{\delta,\varepsilon}(1-\chi^\delta))$$
$$\to \|\varphi^\delta(\chi^\delta) + \varphi^\delta(1-\chi^\delta)\|_{L^2(\Omega_D)} \quad \text{as } \varepsilon \searrow 0.$$

By combining these results, (ii) follows. □

13. GLOBAL EXISTENCE OF SOLUTIONS FOR LOGARITHMIC FREE ENERGIES

Theorem 2 (Global existence in case of logarithmic free energies). *Let the assumptions of Sec.* 10 *hold. Then, there exists a weak solution* (c, μ, χ) *in the sense of Sec.* 4 *of* (1)–(5) *with a logarithmic free energy such that*

(i) $c \in C^{0,1/4}([0,T_0];\ L^2(\Omega;\mathbb{R}^4))$,
(ii) $\partial_t c \in L^2(0,T_0;\ (H_0^1(\Omega;\mathbb{R}^4))')$,
(iii) $\chi \in C^{0,1/2}([0,T_0];\ L^2(\Omega))$,
(iv) $\partial_t \chi \in L^2(0,T_0;\ (H_0^1(\Omega))')$,
(v) *there exists a* $q > 1$ *such that* $\ln c_j \in L^q(\Omega_D)$ *for* $1 \le j \le 4$, $\ln\chi$, $\ln(1-\chi) \in L^2(\Omega_D)$ *and in particular* $0 < \chi, c_j < 1$ *almost everywhere.*

Proof. We pass to the limit $\delta \searrow 0$ in the weak formulation (21)–(23) with f defined by (6) and have to show that (c, μ, χ) found in Lemma 7 is a solution. The limit for (21) can be justified in the same way as in the proof of Theorem 1. To pass to the limit in (22) we must especially take care of the term

$$\chi^\delta \sum_{j=1}^4 \beta_j^1 \varphi^\delta(c_k^\delta) + (1-\chi^\delta)\sum_{j=1}^4 \beta_j^2 \varphi^\delta(c_k^\delta). \tag{41}$$

From the almost everywhere convergence of c_k^δ to c_k, Lemma 8 (i) and the Lemma of Fatou we find

$$\int_{\Omega_{T_0}} \liminf_{\delta\searrow 0} |\varphi^\delta(c_k^\delta)|^q \le \liminf_{\delta\searrow 0} \int_{\Omega_{T_0}} |\varphi^\delta(c_k^\delta)|^q \le C.$$

Next we will show that

$$\lim_{\delta\searrow 0} \varphi^\delta(c_k^\delta) = \begin{cases} \phi(c_k) & \text{if } \lim_{\delta\searrow 0} c_k^\delta = c_k > 0, \\ \infty & \text{if } \lim_{\delta\searrow 0} c_k^\delta = c_k \le 0 \end{cases} \tag{42}$$

almost everywhere in Ω_D. For a point $(x,t) \in \Omega_D$ with $\lim_{\delta\searrow 0} c_k^\delta(x,t) = c_k(x,t)$, we obtain from $\varphi^\delta(d) = \phi(d)$ for $d \ge \delta$ that $\varphi^\delta(c^\delta(x,t)) \to \phi(c(x,t))$. In the second case of a point $(x, t) \in \Omega_D$ with $\lim_{\delta \searrow 0} c_k^\delta(x, t) = c_k(x, t) \le 0$, we have for δ small enough

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

This proves (42). A similar statement holds for $\psi^\delta(\chi^\delta)$.

From (42) and Lemma 8(i) we deduce $0 < c_k < 1$ almost everywhere, $\int_{\Omega_{T_0}} |\phi(c_k)|^q \le C$ and $\varphi^\delta(c_k^\delta) \to \phi(c_k)$ almost everywhere. With Vitali's theorem we find

$$\varphi^\delta(c_k^\delta) \to \phi(c_k) \quad \text{in } L^1(\Omega_D).$$

This allows to pass to the limit in (22).

Let us now consider the limit in (23). The relation $0 < c_k < 1$ almost everywhere implies $\sum_{j=1}^4 \beta_j \psi^\delta(c_j^\delta) \to \sum_{j=1}^4 \beta_j \psi(c_j)$ almost everywhere in Ω_D as in the first case of (42). From $\varphi^\delta(c_k^\delta) \in L^q(\Omega_D)$, the uniform boundedness of χ^δ and Vitali's theorem we infer

$$\chi^\delta \sum_{j=1}^4 \beta_j^1 \psi^\delta(c_j^\delta) \to \chi \sum_{j=1}^4 \beta_j^1 \psi(c_j) \quad \text{in } L^1(\Omega_D).$$

By repeating the argumentation from above for $\varphi^\delta(\chi^\delta) + \varphi^\delta(1-\chi^\delta)$ we deduce $0 < \chi < 1$ almost everywhere in Ω_D which again yields with the help of Vitali's theorem

$$\varphi^\delta(\chi^\delta) + \varphi^\delta(1-\chi^\delta) \to \phi(\chi) + \phi(1-\chi) \quad \text{in } L^1(\Omega_D).$$

So we can also pass to the limit in (23). □

14. UNIQUENESS OF THE SOLUTION

To show uniqueness of problem (1)–(5), we use an integration in time method.

Theorem 3 (Uniqueness of the solution)**.** *Assume that conditions* (17), (18) *and* (19) *hold and that* $\partial_c f, \partial_\chi f$ *are Lipschitz continuous. Then the solution* (c, μ, χ) *of the diffuse interface equations obtained in Theorem* 1 *for polynomial free energy and in Theorem* 2 *for logarithmic free energy is unique in the spaces stated in these theorems.*

Proof. Assume that (c^i, χ^i, μ^i), $i = 1, 2$ are two solutions of system (1)–(5). Now, let $c := c^2 - c^1$, $\chi := \chi^2 - \chi^1$, $\mu := \mu^2 - \mu^1$, $r := r(c^2) - r(c^1)$, $\psi := \partial_\chi f(c^2, \chi^2) - \partial_\chi f(c^1, \chi^1)$.

The difference (c, χ, μ) solves the weak formulation

$$-\int_{\Omega_{T_0}} \partial_t \xi \cdot c + \int_{\Omega_{T_0}} L\nabla\mu : \nabla\xi - \int_{\Omega_{T_0}} r \cdot \xi = 0, \tag{43}$$

$$\int_{\Omega_{T_0}} \left(\partial_c f(c^2, \chi^2) - \partial_c f(c^1, \chi^1)\right) \cdot \eta + \Lambda\nabla c : \nabla\eta = \int_{\Omega_{T_0}} \mu \cdot \eta, \tag{44}$$

$$-\int_{\Omega_{T_0}} \tau \partial_t \zeta \chi + \int_{\Omega_{T_0}} \gamma \nabla\chi \cdot \nabla\zeta - \int_{\Omega_{T_0}} \psi \cdot \zeta = 0. \tag{45}$$

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For given $\eta \in L^2(0, T_0;\ H_0^1(\Omega, \mathbb{R}^4))$ and $t_0 \in (0, T_0)$ we define

$$\xi(\cdot, t) := \begin{cases} \int_t^{t_0} \eta(\cdot, s)ds & \text{if } t \leq t_0, \\ 0 & \text{if } t > t_0. \end{cases} \tag{46}$$

Approach (46) goes back to an idea of Blowey and Elliott (1991). If we use this as a test function in (43) we obtain

$$\begin{aligned} 0 &= \int_{\Omega_{t_0}} c \cdot \eta + \int_{\Omega_{t_0}} L\nabla\mu : \nabla\left(\int_t^{t_0} \eta(s)ds\right) - \int_{\Omega_{t_0}} r \cdot \left(\int_t^{t_0} \eta(s)ds\right) \\ &= \int_{\Omega_{t_0}} c \cdot \eta + \int_{\Omega_{t_0}} L\nabla\left(\int_0^t \mu(s)ds\right) : \nabla\eta - \int_{\Omega_{t_0}} \left(\int_0^t r(s)ds\right) \cdot \eta. \end{aligned} \tag{47}$$

This implies

$$\mathcal{G}\left(c - \int_0^t r(s)ds\right) = -\int_0^t \mu(s)ds \quad \text{and} \quad \partial_t \mathcal{G}\left(c - \int_0^t r(s)\, ds\right) = -\mu.$$

By choosing $\eta := \mu$ in (47) we obtain

$$\begin{aligned} 0 = \int_{\Omega_{t_0}} c \cdot \mu &+ \int_{\Omega_{t_0}} L\nabla\left(\mathcal{G}\left(\int_0^t r(s)ds - c\right)\right) : \nabla\left(\partial_t \mathcal{G}\left(\int_0^t r(s)ds - c\right)\right) \\ &- \int_{\Omega_{t_0}} \left(\int_0^t r(s)ds\right) \cdot \mu \end{aligned}$$

and consequently

$$\begin{aligned} 0 = \int_{\Omega_{t_0}} c \cdot \mu &+ \int_{\Omega} L\nabla\mathcal{G}\left(\int_0^{t_0} r(s)ds - c(t_0)\right) : \nabla\mathcal{G}\left(\int_0^{t_0} r(s)ds - c(t_0)\right) \\ &- \int_{\Omega_{t_0}} \left(\int_0^t r(s)ds\right) \cdot \mu. \end{aligned} \tag{48}$$

In Eq. (44) we test with $\eta := \mathcal{X}_{[0,t_0]}c$. Hence we have

$$\int_{\Omega_{t_0}} c \cdot \mu = \int_{\Omega_{t_0}} \Lambda\nabla c : \nabla c + \left(\partial_c f(c^2, \chi^2) - \partial_c f(c^1, \chi^1)\right) \cdot c. \tag{49}$$

From (48) and (49) we learn

$$\begin{aligned} &\left\| \left(\int_0^{t_0} r\right) - c(t_0) \right\|_L^2 + \int_{\Omega_{t_0}} \Lambda\nabla c : \nabla c - \int_{\Omega_{t_0}} \left(\int_0^t r(s)ds\right) \cdot \mu \\ &\quad = -\int_{\Omega_{t_0}} \left(\partial_c f(c^2, \chi^2) - \partial_c f(c^1, \chi^1)\right) \cdot c. \end{aligned} \tag{50}$$

From the free energy estimate we infer that if conditions (17), (19) and (18) hold, then

$$\int_{\Omega_{t_0}} \left(\int_0^t r(s)ds \right) \cdot \mu \leq 0.$$

Furthermore Λ is positive definite, i.e., there is a constant $\lambda_0 > 0$ such that

$$\int_{\Omega_{t_0}} \Lambda \nabla c : \nabla c \geq \lambda_0 \int_{\Omega_{t_0}} |\nabla c|^2.$$

So we have with (50)

$$\lambda_0 \int_{\Omega_{t_0}} |\nabla c|^2 \leq - \int_{\Omega_{t_0}} \left(\partial_c f(c^2, \chi^2) - \partial_c f(c^1, \chi^1) \right) \cdot c. \tag{51}$$

In (45) we choose the test function $\mathscr{X}_{[0,t_0]}\chi$ analoguos to the setting (46). This leads to

$$\frac{\tau}{\gamma} \int_{\Omega_{t_0}} \chi\eta + \int_{\Omega_{t_0}} \nabla \left(\int_0^t \chi(s)ds \right) : \nabla\eta(t) - \frac{1}{\gamma} \int_{\Omega_{t_0}} \eta(t) \int_0^t \psi(s)ds = 0. \tag{52}$$

This implies because of $\chi(0) = 0$

$$(-\triangle)^{-1} \left(\frac{\tau}{\gamma}\chi - \frac{1}{\gamma} \int_0^t \psi(s)ds \right) = - \int_0^t \chi(s)ds \quad \text{and}$$
$$\partial_t (-\triangle)^{-1} \left(\frac{\tau}{\gamma}\chi - \frac{1}{\gamma} \int_0^t \psi(s)ds \right) = -\chi(t).$$

We set $\eta := \chi$ in (52). As in the treatment of Eq. (43) this yields

$$0 = \gamma\tau \int_{\Omega_{t_0}} |\chi|^2 + \left\| \tau\chi(t_0) - \left(\int_0^{t_0} \psi(s) \right) \right\|_{L^2}^2 - \gamma \int_{\Omega_{t_0}} \chi(t) \int_0^t \psi(s)ds$$

and consequently with Young's inequality

$$\tau \int_{\Omega_{t_0}} |\chi|^2 \leq \delta \int_{\Omega_{t_0}} |\chi|^2 + \frac{C}{\delta} \int_{\Omega_{t_0}} \left(\int_0^t \psi(s)ds \right)^2. \tag{53}$$

Now we add (51) and (53) to find

$$\lambda_0 \int_{\Omega_{t_0}} |\nabla c|^2 + \tau \int_{\Omega_{t_0}} |\chi|^2 \leq \delta C \int_{\Omega_{t_0}} \left(|c|^2 + |\chi|^2 \right)$$
$$+ \frac{C}{\delta} \int_{\Omega_{t_0}} \left(\int_0^t \psi(s)ds \right)^2 + \left| \partial_c f(c^2, \chi^2) - \partial_c f(c^1, \chi^1) \right|^2.$$

For δ small the first integral on the right hand side can be absorbed on the left. As

$$|\partial_c f(c^2, \chi^2) - \partial_c f(c^1, \chi^1)|^2 + |\partial_\chi f(c^2, \chi^2) - \partial_\chi f(c^1, \chi^1)|^2 \leq C_0 \left(|c|^2 + |\chi|^2 \right)$$

where C_0 depends on the Lipschitz constant of $\partial_c f$ and $\partial_\chi f$, we find at last by exploiting the Poincaré inequality

$$\int_{\Omega_{t_0}} \left(|\nabla c|^2 + |\chi|^2\right) \leq C \int_{\Omega_{t_0}} |\nabla c|^2 + |\chi|^2 + \int_0^t \int_{\Omega_{t_0}} \left(|\nabla c|^2 + |\chi|^2\right).$$

With Gronwall's inequality this finally means $c = \chi = 0$ in Ω_{t_0} and with (44) $\mu = 0$ in Ω_{t_0}. By repeating the argument, since $t_0 > 0$, this holds in the whole of Ω_D. □

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