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Global solution to a phase transition problem of the Allen-Cahn type

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1 Introduction

In the talk given by the first author, a model of phase segregation of the Allen-Cahn type was presented [5]. This model leads to a system of two differential equations, one partial the other ordinary, respectively interpreted as balances of microforces and microenergy. The two unknowns are the order parameter entering the standard Allen-Cahn equation and the chemical potential. This system has been extensively studied in [1]: the results will be recalled in this presentation.

A notion of maximal solution to the o.d.e., parameterized on the order-parameter field, is given. By substitution in the p.d.e. of the so-obtained chemical potential field, the latter equation takes the form of an Allen-Cahn equation for the order parameter, with a memory term. Existence and uniqueness of global-in-time smooth solutions to this modified Allen-Cahn equation can be shown along with a description of the relative ω-limit set.

2 Setting of the problem

We deal with a system of evolution equations, given by the microforce balance and the energy balance, respectively,

$$\kappa\,\partial_t\rho - \Delta\rho + f'(\rho) = \mu \tag{2.1}$$

and

$$\partial_t(-\mu^2\rho) = \mu\left(\kappa\,(\partial_t\rho)^2 + \bar{\sigma}\right) \tag{2.2}$$

in terms of the unknowns ρ and μ. It is a nonlinear system consisting of a parabolic PDE and a first-order-in-time ODE, to be solved for the order-parameter field ρ and the chemical potential field μ. In particular, $\rho = \rho(x,t) \in [0,1]$ can be interpreted as the scaled volumetric density of one of the two phases, $\kappa > 0$ is a *mobility* coefficient, and f denotes a double-well potential confined in $(0,1)$ and singular at endpoints. Moreover, in (2.2) $\bar{\sigma} = \bar{\sigma}(x, t$ represents a source term which is assumed to be a datum of the problem. Formally, setting $\mu \equiv 0$ in (2.1) restitutes the standard Allen-Cahn equation (see [2, 3, 4] for classes of related models).

System (2.1)–(2.2) is complemented with the homogeneous Neumann condition

$$\partial_n\rho = 0 \quad \text{on the body's boundary} \tag{2.3}$$

(here ∂_n denotes the outward normal derivative) and with the initial conditions

$$\rho|_{t=0} = \rho_0 \quad \text{bounded away from } 0\,, \quad \mu|_{t=0} = \mu_0 \geq 0\,. \tag{2.4}$$

We point out that the quantity $\eta = -\mu^2\rho$ representing the microentropy cannot exceed the level 0 from below, and that the corresponding prescribed initial field

$$\eta|_{t=0} = \eta_0 = -\mu_0^2\rho_0 \tag{2.5}$$

is nonpositive-valued.

3 Solution strategy and summary of results

The aim is a mathematical investigation of problem (2.1)–(2.4). We try to discuss the ODE first, then to solve the PDE. In order to carry out our strategy, we introduce a change of variable to give (2.2) plus (2.5) the form of a parametric initial-value problem. We set

$$\xi := -\eta, \quad \xi_0 := -\eta_0, \tag{3.1}$$

whence $\mu = \sqrt{\xi/\rho}$ and ξ should satisfy

$$\partial_t\xi + \frac{\kappa\,(\partial_t\rho)^2 + \bar{\sigma}}{\sqrt{\rho}}\,\sqrt{\xi} = 0, \quad \xi|_{t=0} = \xi_0, \tag{3.2}$$

that is, a Cauchy problem parameterized on the space variable x and on the field $\rho(x,\cdot)$. The general form of equation (3.2) entails the Peano phenomenon and allows the existence of infinitely many solutions; among them, we pick a suitably defined *maximal solution* ξ (or $\sqrt{\xi}$), having the desirable property to stay positive as long as is possible. Next, we transform (2.1) into

$$\kappa\,\partial_t\rho - \Delta\rho + f'(\rho) - \sqrt{\xi}\frac{1}{\sqrt{\rho}} = 0, \tag{3.3}$$

that is, an Allen-Cahn equation for ρ with the additional term $-\sqrt{\xi/\rho}$. Note that the factor $\sqrt{\xi}$ is implicitly defined in terms of ρ as the maximal solution to (3.2). Then, (3.3) may be viewed as an *integrodifferential equation*. Existence, regularity and uniqueness of the solution to (3.3) subject to the boundary condition (2.3) and the initial condition $(2.4)_1$ are proved by using a fixed-point argument, which takes advantage of the iterated Contraction Mapping Principle. What is important for our procedure is the a priori uniform boundedness of $\partial_t\rho$ in the space-time domain; this is shown by applying standard regularity arguments for parabolic equations.

Our analysis is also devoted to an investigation of the long-time behavior of the solution: it turns out that $\sqrt{\xi}$ uniquely converges to some function φ_∞ and any element ρ_∞ of the $\omega-$limit set solves the stationary problem

$$-\Delta\rho_\infty + f'(\rho_\infty) - \varphi_\infty\frac{1}{\sqrt{\rho_\infty}} = 0, \tag{3.4}$$

supplemented by suitable homogeneous Neumann boundary conditions.

4 Discussion of the model

Let us start from the Allen-Cahn equation

$$\kappa\,\partial_t\rho - \Delta\rho + f'(\rho) = 0, \tag{4.1}$$

which has been introduced to describe evolutionary processes in a two-phase material body, including *phase segregation*: indeed, the *order-parameter* field ρ may represent a density of one of the two phases and f is usually a double-well potential playing in a fixed range of significant values for the order paramenter, say $[0,1]$. The derivation of (4.1) proposed by Gurtin [3] is based on a *balance of contact and distance microforces*:

$$\operatorname{div}\boldsymbol{\xi} + \pi + \gamma = 0 \tag{4.2}$$

along with a *dissipation inequality* restricting the free-energy growth:

$$\partial_t\psi \le w, \quad w := -\pi\,\partial_t\rho + \boldsymbol{\xi}\cdot\nabla(\partial_t\rho), \tag{4.3}$$

where the distance microforce is split in an internal part π and an external part γ, the vector $\boldsymbol{\xi}$ denotes the *microscopic stress*, and w specifies the (distance and contact) internal microworking. Similarly, in [2] the balance of microforces is stated under form of a principle of virtual power for microscopic motions. The Coleman-Noll compatibility of the constitutive choices

$$\pi = \widehat{\pi}(\rho, \nabla\rho, \partial_t\rho), \quad \boldsymbol{\xi} = \widehat{\boldsymbol{\xi}}(\rho, \nabla\rho, \partial_t\rho),$$
$$\text{and} \quad \psi = \widehat{\psi}(\rho, \nabla\rho) = f(\rho) + \frac{1}{2}|\nabla\rho|^2 \tag{4.4}$$

with the dissipation inequality (4.3) yields

$$\widehat{\pi}(\rho, \nabla\rho, \partial_t\rho) = -f'(\rho) - \widehat{\kappa}(\rho, \nabla\rho, \partial_t\rho)\partial_t\rho, \quad \widehat{\boldsymbol{\xi}}(\rho, \nabla\rho, \partial_t\rho) = \nabla\rho. \tag{4.5}$$

Hence, the Allen-Cahn equation (4.1) follows for $\widehat{\kappa}(\rho, \nabla\rho, \partial_t\rho) = \kappa$ and $\gamma \equiv 0$.

In [5] the third author considered a modified version of Gurtin's derivation, in which inequality (4.3) is dropped and the microforce balance (4.2) is coupled both with the *microenergy balance*

$$\partial_t\varepsilon = e + w, \quad e := -\operatorname{div}\bar{\boldsymbol{h}} + \bar{\sigma}, \tag{4.6}$$

and the *microentropy imbalance*

$$\partial_t\eta \geq -\operatorname{div}\boldsymbol{h} + \sigma, \quad \boldsymbol{h} := \mu\bar{\boldsymbol{h}}, \quad \sigma := \mu\bar{\sigma}. \tag{4.7}$$

In this approach to phase-segregation modeling, it is postulated that the *microentropy inflow* $(\boldsymbol{h}, \sigma)$ is proportional to the *microenergy inflow* $(\bar{\boldsymbol{h}}, \bar{\sigma})$ through the *chemical potential* μ, *a positive field.* Consistently, the free energy is defined to be

$$\psi := \varepsilon - \mu^{-1}\eta, \tag{4.8}$$

with the chemical potential playing the same role as *coldness* in the deduction of the heat equation. Just as absolute temperature turns out a macroscopic measure of microscopic *agitation*, its inverse - the coldness - measures microscopic *quiet.* Likewise, the chemical potential can be seen as a macroscopic measure of microscopic *organization.* Combination of (4.6)–(4.8) yields

$$\partial_t\psi \leq -\eta\partial_t(\mu^{-1}) + \mu^{-1}\bar{\boldsymbol{h}} \cdot \nabla\mu - \pi\,\partial_t\rho + \boldsymbol{\xi} \cdot \nabla(\partial_t\rho), \tag{4.9}$$

an inequality that restricts constitutive choices: however, these can now be more general than those in (4.4).

Now, assume that the constitutive mappings delivering π, ξ, η, and $\bar{\boldsymbol{h}}$ depend on the list $\rho, \nabla\rho, \partial_t\rho$, *and* the chemical potential μ. Then choose

$$\psi = \widehat{\psi}(\rho, \nabla\rho, \mu) = -\mu\,\rho + f(\rho) + \frac{1}{2}|\nabla\rho|^2, \tag{4.10}$$

and observe that compatibility with (4.9) implies

$$\begin{aligned} \widehat{\pi}(\rho, \nabla\rho, \partial_t\rho, \mu) &= \mu - f'(\rho) - \widehat{\kappa}(\rho, \nabla\rho, \partial_t\rho)\partial_t\rho, \quad \widehat{\boldsymbol{\xi}}(\rho, \nabla\rho, \partial_t\rho, \mu) = \nabla\rho, \\ \widehat{\eta}(\rho, \nabla\rho, \partial_t\rho, \mu) &= -\mu^2\rho, \quad \widehat{\bar{\boldsymbol{h}}}(\rho, \nabla\rho, \partial_t\rho, \mu) \equiv \boldsymbol{0}. \end{aligned} \tag{4.11}$$

In view of (4.11) and under the additional constitutive assumptions that the mobility κ is a positive constant and the external distance microforce γ is null, the microforce balance (4.2) and the energy balance (4.6) become, respectively, (2.1) and (2.2).

5 Precise statement of results

Here, we mainly refer to the system of equations in (3.3) and (3.2), which are derived from (2.1) and (2.2) via the transformation (3.1). Let Ω be a smooth bounded domain of $\mathbb{R}^N (N \geq 1)$ with boundary Γ and take the space time domains $Q_t := \Omega \times [0, t)$, $t \in (0, +\infty]$). As to the *coarse-grain free energy* f, we split it as

$$0 \leq f = f_1 + f_2, \quad \text{where} \quad f_1, f_2 : (0,1) \to \mathbb{R} \quad \text{are } C^2\text{-functions,}$$
$$f_1 \text{ is convex,} \quad f_2' \text{ is bounded,} \quad \lim_{r \searrow 0} f'(r) = -\infty, \quad \text{and} \quad \lim_{r \nearrow 1} f'(r) = +\infty.$$

Actually, a nice example for f_1 is

$$f_1(r) = r \ln r + (1-r)\ln(1-r) \quad \text{for } r \in (0,1),$$

while f_2 stands for a smooth perturbation of this singular convex part. For the energy source $\bar{\sigma}$ and the initial data ρ_0, ξ_0 we assume that

$$\bar{\sigma} \in L^2(Q_T), \quad \rho_0, \xi_0 \in L^\infty(\Omega), \quad 0 < \rho_0 < 1 \quad \text{and} \quad \xi_0 \geq 0 \quad \text{a.e. in } \Omega.$$

and recall that the mobility κ is a given positive constant.

Consider now the forward Cauchy problem (3.2). Clearly, ξ must be nonnegative. Thus, if we look for a strictly positive ξ (for given $\rho > 0$ and $\xi_0 > 0$), the Cauchy problem (3.2) admits a unique local solution. On the contrary, uniqueness is no longer guaranteed if we allow ξ to be just nonnegative. On the other hand, every nonnegative local solution can be extended to a global solution. Therefore, we select a (global) solution to problem (3.2) according to the following *maximality criterion*:

$$\sqrt{\xi(x,t)} = \sup\{w(x,t) : w \in \mathcal{S}^*(\bar{\sigma}, \xi_0, \rho)\} \quad \text{for } (x,t) \in Q_T, \quad \text{where} \tag{5.1}$$
$$\mathcal{S}^*(\bar{\sigma}, \xi_0, \rho) := \Big\{ w \in W^{1,1}(0,T; L^1(\Omega)) : w(0) = \sqrt{\xi_0}, \quad w \geq 0 \quad \text{a.e. in } Q_T,$$
$$\partial_t w = -\big(\kappa (\partial_t \rho)^2 + \bar{\sigma}\big)/(2\rho^{1/2}) \quad \text{a.e. where } w > 0 \Big\}.$$

Accordingly, the maximal ξ satisfies:

$$\sqrt{\xi(x,t)} = \sqrt{\xi_0(x)} - \int_0^t a^*(x,s)\, ds,$$

where

$$a^*(x,s) := \begin{cases} \dfrac{\kappa |\partial_t \rho(x,s)|^2 + \bar{\sigma}(x,s)}{2\sqrt{\rho(x,s)}} & \text{if } \xi(x,s) > 0, \\ 0 & \text{otherwise.} \end{cases}$$

Then, if we replace μ by $\sqrt{\xi/\rho}$ in (2.1), we get (3.3). We supplement this equation with the boundary and initial conditions for ρ given by, respectively, (2.3) and the first of (2.4). Of the so-obtained initial/boundary value problem, a variational formulation in the framework of the spaces $V := H^1(\Omega)$ and $H := L^2(\Omega)$ is:

$$\text{look for } \rho \in H^1(0,T;H) \cap C^0([0,T];V) \text{ such that} \tag{5.2}$$

$$\rho(0) = \rho_0, \quad 0 < \rho < 1 \quad \text{a.e. in } Q_T, \quad \frac{1}{\rho} + \frac{1}{1-\rho} \in L^\infty(Q_T); \tag{5.3}$$

$$\kappa \int_\Omega \partial_t \rho(t)\, z + \int_\Omega \nabla\rho(t) \cdot \nabla z + \int_\Omega f'(\rho(t))\, z - \int_\Omega \left(\xi(t)/\rho(t)\right)^{1/2} z = 0$$
$$\text{for a.a. } t \in (0,T), \text{ for every } z \in V, \text{ and for } \xi \text{ given by (5.1).} \tag{5.4}$$

The initial-boundary value problem (5.2)–(5.4) can be regarded as an essentially integrodifferential Allen-Cahn equation in the sole unknown ρ. We note, in particular, that (5.4) has a well defined meaning, because $\xi^{1/2} \in L^2(Q_T)$ and $\rho^{-1/2} \in L^\infty(Q_T)$ (at least) whenever ρ satisfies (5.2) and $\bar\sigma \in L^2(Q_T)$.

Our first result concerns existence and uniqueness of the solution.

Theorem 5.1 (Well–posedness). *Under the already specified assumptions on the data* f, $\bar\sigma$, ρ_0, ξ_0, *if moreover*

$$\bar\sigma \in L^\infty(Q_\infty) \quad \text{and} \quad \bar\sigma^- \in L^1(0,\infty;L^\infty(\Omega)); \quad \frac{1}{\rho_0} + \frac{1}{1-\rho_0} \in L^\infty(\Omega),$$
$$\rho_0 \in H^2(\Omega), \quad \partial_n \rho_0 = 0 \quad \text{on } \Gamma, \quad \text{and} \quad \Delta\rho_0 \in L^\infty(\Omega),$$

then, for every $T \in (0,+\infty)$, *problem* (5.2)–(5.4) *has a unique solution. Furthermore,*

$$\rho \in L^p(0,T;W^{2,p}(\Omega)) \quad \text{for every } p < +\infty,$$
$$\partial_t\rho \in L^\infty(Q_T), \quad \text{and} \quad \xi \in L^\infty(Q_T). \tag{5.5}$$

Finally, there exist constants $\rho_*, \rho^* \in (0,1)$ *and* $\xi^* \geq 0$, *independent of* T, *such that*

$$\rho_* \leq \rho \leq \rho^*, \quad \xi \leq \xi^* \quad \text{a.e. in } Q_T. \tag{5.6}$$

Our second result deals with the long-time behavior of the solution ρ to problem (5.2)–(5.4) and ensures that the elements of the ω-limit of every trajectory are steady states. Let us describe the stationary problem associated to (5.2)–(5.4). We introduce $\varphi_\infty : \Omega \to [0,+\infty)$ defined by

$$\varphi_\infty(x) := \lim_{t\to+\infty} \sqrt{\xi(x,t)} \quad \text{for a.a. } x \in \Omega, \quad \text{where } \sqrt{\xi} \text{ is given by (5.1)}$$

notice that the stationary problem reads:

$$\text{find } \rho_\infty \in V \text{ such that } \rho_* \leq \rho_\infty \leq \rho^* \quad \text{a.e. in } \Omega \quad \text{and} \tag{5.7}$$

$$\int_\Omega \nabla\rho_\infty \cdot \nabla z + \int_\Omega f'(\rho_\infty)\, z - \int_\Omega \frac{\varphi_\infty}{\sqrt{\rho_\infty}}\, z = 0 \quad \text{for every } z \in V. \tag{5.8}$$

Theorem 5.2 (Structure of ω-limit). *Under the same assumptions as in Theorem 5.1, let* ρ *be the unique global solution to problem* (5.2)–(5.4). *Then, the limit* $\varphi_\infty(x)$ *exists for a.a.* $x \in \Omega$ *and* $\varphi_\infty \in L^\infty(\Omega)$. *Moreover, the* ω*-limit defined by*

$$\omega(\rho) := \{\rho^\infty \in H : \ \rho^\infty = \lim_{n\to\infty} \rho(t_n) \text{ strongly in } H \text{ for some } \{t_n\} \nearrow +\infty\} \tag{5.9}$$

is non-empty, compact, and connected in the strong topology of H. *Finally, every element* $\rho^\infty \in \omega(\rho)$ *coincides with a solution* ρ_∞ *to the stationary problem* (5.7)–(5.8).

For the detailed proofs of Theorems 5.1 and 5.2, as well as for an informal discussion of the employed techniques, we refer the reader to [1].

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