Instituto de Matemática, Estatística e
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Modelos do Tipo Campo de Fases em Processos de Cristalização

Patrícia Nunes da Silva

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Prof. Dr.: José Luiz Boldrini
Orientador

Banca Examinadora:

1. Prof. Dr. José Luiz Boldrini
2. Prof. Dr. Arnaldo Simal do Nascimento
3. Prof. Dr. Gustavo Perla Menzala
4. Prof. Dr. Marcelo Martins dos Santos
5. Prof. Dr. Marko Antonio Rojas Medar

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Prof (a). Dr (a). JOSÉ LUIZ BOLDRINI

Prof (a). Dr (a). MARKO ANTONIO ROJAS MEDAR

Prof (a). Dr (a). MARCELO MARTINS DOS SANTOS

Prof (a). Dr (a). GUSTAVO ALBERTO PERLA MENZALA

Prof (a). Dr (a). ARNALDO SIMAL DO NASCIMENTO

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Conteúdo

Resumo

Neste trabalho apresentamos alguns resultados de existência de solução para sistemas de equações diferenciais parciais não lineares consistindo de uma equação do tipo Cahn-Hilliard e várias equações do tipo Allen-Cahn. Tais sistemas são análogos ao modelo proposto por Fan, L.-Q. Chen, S. Chen e Voorhees a fim de modelar o fenômeno "Ostwald ripening" em sistemas bifásicos. Utilizamos o método de Faedo-Galerkin e argumentos de compacidade a fim de obter resultados de existência e unicidade de soluções fracas.

Abstract

We analyze a family of systems consisting of a Cahn-Hilliard and several Allen-Cahn type equations. These systems are analogous to one proposed by Fan, L.-Q. Chen, S. Chen and Voorhees for modeling Ostwald ripening in two-phase systems. We prove results on existence and uniqueness of weak solutions by using the Faedo-Galerkin method and compactness arguments.

Introdução

"Ostwald ripening" é o nome que se dá a um processo de evolução microestrutural que tem sido comumente observado em uma ampla gama de sistemas bifásicos. Devido à sua grande importância prática em vários campos de aplicação, que incluem por exemplo indústrias de fundição, processos de soldagem, e vários outros processos industriais, este mecanismo de crescimento cristalino tem sido bastante estudado (veja, por exemplo, Tavare [8]).

Trata-se basicamente de um mecanismo de crescimento de cristais de uma certa fase quando dispersa em uma matriz de outra fase. Observa-se experimentalmente que durante tal processo o tamanho médio da fase dispersa geralmente cresce devido à difusão através da fase da matriz, o que é em geral acompanhado de uma diminuição do número inicial de partículas cristalinas da fase dispersa.

Do ponto de vista físico, sabe-se que o mecanismo que controla a evolução deste fenômeno está relacionado à redução da área interfacial total, o que implica que a energia interna total sistema tende a decrescer. Observa-se também que tal energia pode depender, além da estrutura geométrica das interfaces, da sua orientação cristalográfica.

Do ponto de vista da modelagem matemática, um procedimento comum é modelar este tipo de fenômeno de forma a que ele seja governado por equações parciais que descrevem adequadamente o mecanismo de difusão do soluto (fase dispersa) na fase da matriz, acopladas a equações que regem o desenvolvimento das interfaces e que regulam a troca espacial de material. Entretanto, como as regiões correspondentes às diversas fases não são conhecidas a priori, o estudo das soluções de tais sistemas de equações (em seus vários aspectos, tanto teóricos quanto numéricos) em geral inclui questões relativas a problemas de fronteira livre e são de análise e simulação numérica bastante complicadas. Em outras palavras, um aspecto bastante difícil deste tipo de problema é o do modelamento adequado da interface entre as fases. Uma alternativa bastante promissora ao enfoque que introduz uma interface que funciona como fronteira livre e na qual há descontinuidade nos valores de certas propriedades físicas (o que leva aos chamados problemas do tipo Stefan), é a de utilizar os chamados modelos de campos de fase ("phase field models"). Estes são modelos contínuos que permitem que as interfaces tenham espessura e estrutura interna. Isso é obtido pela utilização de certas variáveis, com o nome genérico de campos de fases ("phase fields"), de tal forma que as interfaces são dadas por superfícies de nível adequadas destas funções. Como referência histórica, lembramos que o primeiro modelo de campo de fases para o estudo da transição sólido/líquido foi proposto por Langer [7] (veja também Caginalp [1]).

Formulações nestes termos são bastante convenientes para a computação de situações realistas envolvendo interfaces de estrutura complicada, tais como os chamados crescimentos dendríticos (veja, por exemplo, Caginalp e Socolovsky [2]). Outra vantagem deste tipo de modelo é a de que eles são embasados na termodinâmica (inclusive irreversível) subjacente ao fenômeno.

Neste trabalho, estudamos um sistema de equações diferenciais parciais não lineares formado pelo acoplamento de uma equação parabólica não linear de quarta ordem e várias de segunda ordem. Mais especificamente, temos o acoplamento de uma equação do tipo Cahn-Hilliard e várias do tipo Allen-Cahn. Este tipo de sistema foi introduzido por Cahn e Novick-Cohen [4] como uma extensão dos trabalhos originalmente apresentados por Cahn e Hilliard [3, 5]. Tal extensão permitiu a modelagem da ocorrência simultânea dos fenômenos de separação de fases e de ordenação. Tal posssibilidade responde a um dos maiores interesses no estudo cristalográfico de ligas: a estrutura ou regularidade da distribuição das partículas no espaço. Em nosso caso, o sistema proposto por Fan et al. [6] lança mão da descrição através de campos de fase a fim de modelar o crescimento de cristais levando em conta a complexidade da evolução microestrutural e a difusão *long-range* em materiais bifásicos simultaneamente.

A apresentação dos capítulos segue a ordem cronológica de desenvolvimento da pesquisa. No Capítulo 1, obtemos um resultado de existência e unicidade de solução para uma família de sistemas relacionados ao sistema proposto por Fan et al. [6]. No Capítulo 2, obtemos existência e unicidade de uma solução generalizada para o modelo proposto por Fan et al. [6]. No Capítulo 3, melhoramos a regularidade da solução obtida no Capítulo 1. No Capítulo 4, apresentamos uma nova família de sistemas também relacionados ao sistema proposto por Fan et al. [6] para a qual apresentamos resultados de existência e unicidade de solução com a mesma regularidade da solução obtida no Capítulo 3. Para efeito de completude, no Capítulo 5, apresentamos resultados de existência e unicidade de solução para o modelo proposto por Fan et al. [6] quando temos a limitação inferior da densidade de energia livre local associada ao sistema. Terminamos a apresentação compilando os resultados obtidos neste trabalho e discutindo o desenvolvimento da pesquisa.

Capítulo 1

Existência e Soluções Aproximadas de um Modelo para "Ostwald Ripening"

Resumo

Utilizando um esquema de elementos finitos baseado no método de Euler atrasado, analisamos uma discretização completa de um sistema formado por uma equação do tipo Cahn-Hilliard e várias do tipo Allen-Cahn. Tal sistema foi proposto por Fan, L.-Q. Chen, S. Chen e Voorhees para modelar o fenômeno de "Ostwald ripening" em sistemas de duas fases. Como conseqüência desta análise, provamos a existência e unicidade das soluções dos problemas discretos bem como a convergência destas soluções para a solução do problema original.

Existence and Approximate Solutions of a Model for Ostwald Ripening

Patrícia Nunes da Silva
nunes@ime.unicamp.br

José Luiz Boldrini
boldrini@ime.unicamp.br

Abstract

We analyze a fully discrete finite element scheme based on the backward Euler method for a system consisting of a Cahn-Hilliard and several Allen-Cahn type equations. This system was proposed by Fan, L.-Q. Chen, S. Chen and Voorhees for modeling Ostwald ripening in two-phase systems. As a consequence of the analysis, we prove the existence and uniqueness of solutions of the discrete problems, as well as their convergence to the solution of the original system.

1.1 Introduction

Ostwald ripening is a phenomenon observed in a wide variety of two-phase systems in which there is coarsening of one phase dispersed in the matrix of another. Because its practical importance, this process has been extensively studied in several degrees of generality. In particular for Ostwald ripening of anisotropic crystals, Fan, Chen, Chen & Voorhees (1998) presented a model taking in consideration both the evolution of the compositional field and of the crystallographic orientations. In the work of Fan et al. (1998), there are also numerical experiments used to validate the model, but there is no rigorous mathematical analysis of the model.

Our objective in this paper is to do such mathematical analysis for a family of models of Ostwald ripening related to that presented by Fan et al. (1998). Such family is constituted of the following Cahn-Hilliard and Allen-Cahn equations:

$$\partial_t c = \Delta w, \tag{1.1}$$

$$w = D\Big[\partial_c \mathcal{F} - \lambda_c \Delta c\Big], \tag{1.2}$$

$$\partial_t \theta_i = -L_i\Big[\partial_{\theta_i} \mathcal{F} - \lambda_i \Delta \theta_i\Big], \qquad i = 1, \dots, p, \tag{1.3}$$

subject to the initial conditions

$$c(x,0) = c_0(x), \qquad x \in \Omega, \tag{1.4}$$
$$\theta_i(x,0) = \theta_{i0}(x), \qquad x \in \Omega, \qquad i = 1, \dots, p \tag{1.5}$$

and boundary conditions

$$\frac{\partial c}{\partial n} = \frac{\partial w}{\partial n} = 0 \quad \text{on } \partial\Omega, \tag{1.6}$$
$$\frac{\partial \theta_i}{\partial n} = 0 \quad \text{on } \partial\Omega, \quad \text{for } i = 1, \dots, p. \tag{1.7}$$

Here, Ω is the physical region where the Ostwald process is occurring; $c(x,t)$, for $t \in [0,T]$, $0 < T < +\infty$, $x \in \Omega$, is the compositional field (fraction of the soluto with respect to the mixture); $\theta_i(x,t)$, for $i = 1, \dots, p$, are the crystallographic orientations fields; D, λ_c, L_i, λ_i are positive constants related to the material properties and $\frac{\partial}{\partial n}$ denotes the exterior normal derivative at the boundary. The function $\mathcal{F} = \mathcal{F}(c, \theta_1, \dots, \theta_p)$ is the local free energy density whose exact form will be presented in the next section.

We analyze a fully discrete finite element scheme based on the backward Euler method for a model closely related to that presented by Fan et al. (1998). In this analysis, we show that the approximate solutions converge to a solution of the original continuous model and this, in particular, will furnish a rigorous proof of the existence of weak solutions (see the statement of Theorem 1.1). Our approach is similar to that used by Copetti & Elliott (1992) for the Cahn-Hilliard equation (with logarithm singularity in the free energy).

1.2 Technical hypotheses and existence of solutions

Throughout this paper, we assume that Ω is a bounded domain in R^d, $1 \le d \le 3$, which has Lipschitz boundary. Standard notation will be used for the required functional spaces.

Similarly as in Fan et al. (1998), it is assumed that the local free energy $\mathcal{F}$ has the following form:

$$\begin{aligned}\mathcal{F}(c, \theta_1, \dots, \theta_p) = &-\frac{A}{2}(c - c_m)^2 + \frac{B}{4}(c - c_m)^4 + \frac{D_\alpha}{4}(c - c_\alpha)^4 \\ &+ \frac{D_\beta}{4}(c - c_\beta)^4 - \gamma \sum_{i=1}^{p} g(c, \theta_i) + \frac{\delta}{4}\sum_{i=1}^{p} \theta_i^4 + \sum_{i=1}^{p} \sum_{i \neq j=1}^{p} \varepsilon_{ij} f(\theta_i, \theta_j).\end{aligned} \tag{1.8}$$

A, B, D_α, D_β, γ, δ , ε_{ij}, $i \neq j = 1, \dots, p$, are positive constants related to the material properties, c_α and c_β are the solubilities or equilibrium concentrations for the matrix phase and second phase, respectively, and $c_m = (c_\alpha + c_\beta)/2$.

Functions f and g are assumed to satisfy the following properties:

$$\begin{aligned} &\Big| f(a,b) - f(u,v) + \nabla f(u,v) \cdot (u-a, v-b) \Big| \\ &\qquad \leq F_1 (u-a)^2 + F_2 (v-b)^2 \left(\leq \max\{F_1, F_2\} |(u,v) - (a,b)|^2 \right) \end{aligned} \tag{1.9}$$

and

$$\Big| g(a,b) - g(u,v) + \nabla g(u,v) \cdot (u-a, v-b) \Big| \leq G_1 (u-a)^2 + G_2 (v-b)^2 \tag{1.10}$$

for all $(u,v), (a,b) \in \mathbb{R}^2$ and fixed constants $F_1, F_2, G_1, G_2 \geq 0$. We remark that the previous assumptions on the functions f and g imply that the difference between $f(a,b)$ and $g(a,b)$ and their Taylor polynomials of degree one at (u,v), respectively, are bounded up to a multiplicative fixed constant by the square of the Euclidean distance between (u,v) and (a,b).

We also remark that the local free energy $\mathcal{F}$ is assumed to have form like the one stated above in order to comply to a requirement of Chen & Fan (1996) - Chen, Fan & Geng (1997) that it should have $2p$ degenerate minima at the equilibrium concentration c_β to distinguish the $2p$ orientations differences of the second phase grains in space.

The results of this work apply, for instance, to a family of problems which contains a local free energy density given as in (1.8) but with

$$g(c, \theta_i) = g_{c_\beta}(c - c_\alpha) g_2(\theta_i) \qquad \text{and} \qquad f(\theta_i, \theta_j) = g_2(\theta_i) g_2(\theta_j)$$

where the functions g_M, $M = 2$ or c_β, are given by

$$g_M(u) = u^2 \quad \text{for } |u| \leq M \quad \text{and} \quad g_M(u) = 6M^2 - \frac{8M^3}{|u|} + \frac{3M^4}{|u|^2} \quad \text{for } |u| \geq M.$$

This example coincides in a ball of radius $\min\{c_\beta, 2\}$ with the local free energy density presented by Fan et al. (1998), having therefore the same local minima and satisfying the cited requirement.

We denote by $\overline{w}$, the difference between a function w and its average, that is

$$\overline{w} = w - \frac{1}{|\Omega|} \int_\Omega w dx.$$

Under the previous hypotheses we will prove the following:

THEOREM 1.1 Given $c_0, \theta_{10}, \ldots, \theta_{p0} \in H^1(\Omega)$, there exist unique functions $c, w, \theta_1, \ldots, \theta_p$ such that $c(\cdot, 0) = c_0(\cdot)$, $\theta_i(\cdot, 0) = \theta_{i0}(\cdot)$ and

$$c \in L^\infty(0,T,H^1(\Omega)), \quad \partial_t c \in L^2(0,T,[H^1(\Omega)]') \text{ and } \sqrt{t}\partial_t c \in L^2(0,T,H^1(\Omega))$$
$$\sqrt{t}w \in L^\infty(0,T,H^1(\Omega)),$$
$$\theta_i \in L^\infty(0,T,H^1(\Omega)), \quad \partial_t\theta_i \in L^2(0,T,[H^1(\Omega)]') \text{ and } \sqrt{t}\partial_t\theta_i \in L^2(0,T,H^1(\Omega)),$$
$$\partial_c\mathcal{F}(c,\theta_1,\ldots,\theta_p), \quad \partial_{\theta_i}\mathcal{F}(c,\theta_1,\ldots,\theta_p) \in L^\infty(0,T,L^2(\Omega)),$$

for $i = 1, \ldots, p$, and such that for all $\eta, \pi_i \in C([0,T]; H^1(\Omega))$ there hold

$$\int_0^T \Big(\langle \partial_t c, \eta\rangle + (\nabla \overline{w}, \nabla\eta)\Big)dt = 0, \tag{1.11}$$

$$\int_0^T \Big[\Big(w - D\partial_c\mathcal{F}(c,\theta_1,\ldots,\theta_p),\eta\Big) - D\lambda_c(\nabla c, \nabla\eta)\Big]dt = 0, \tag{1.12}$$

$$\int_0^T \Big[\langle \partial_t\theta_i, \pi_i\rangle + L_i\Big(\partial_{\theta_i}\mathcal{F}(c,\theta_1,\ldots,\theta_p),\pi_i\Big) + L_i\lambda_i(\nabla\theta_i, \nabla\pi_i)\Big]dt = 0, \tag{1.13}$$

for $i = 1, \ldots, p$ and where $\langle\cdot,\cdot\rangle$ denotes the duality pairing between $H^1(\Omega)$ and its dual and $(\cdot,\cdot)$ denotes the inner product in $L^2(\Omega)$.

We remark that equation (1.11) implies that the average of c is conserved.

We also remark that the whole sequence of approximate solutions to be constructed in the next section converges in a suitable sense to the solution of (1.11)–(1.13) (see the statement of Theorem 1.3 for details.)

For sake of simplicity of exposition, in the next sections, we consider only two orientations field variables. The presented results are straightforward extended to any number of such variables.

1.3 Discretization and approximate solutions

To obtain approximate solutions, let us consider $\mathcal{T}^h$ a quasi-uniform family of triangulations of Ω, $\Omega = \cup_{\tau\in\mathcal{T}^h}\tau$, with mesh size h. Let $S^h \subset H^1(\Omega)$ be the finite element space of continuous functions on $\overline{\Omega}$ which are linear on each $\tau \in \mathcal{T}^h$. Denote by $\{x_i\}_{i=1}^N$ the set of nodes of $\mathcal{T}^h$ and let $\{\chi_i\}_{i=1}^N$ be the basis of S^h defined by $\chi_i(x_j) = \delta_{ij}$. We indicate by

$(\cdot,\cdot)$ and by $|\cdot|$ the inner product and the norm in $L^2(\Omega)$ respectively and by $|\cdot|_1$ the seminorm $|\nabla\cdot|$.

Let $k = \frac{T}{N}$ denote the time step where N is a given positive integer. Recalling that we took $p = 2$, the finite element problem corresponding to (1.1)–(1.7) becomes to find $C^n, W^n, \Theta_1^n, \Theta_2^n \in S^h$, $n = 1, \ldots, N$ such that $\forall \chi, \mu_1, \mu_2 \in S^h$,

$$(\partial C^n, \chi) + (\nabla W^n, \nabla\chi) = 0 \tag{1.14}$$

$$(W^n, \chi) = D\Big(\partial_c \mathcal{F}(C^n, \Theta_1^n, \Theta_2^n), \chi\Big) + \lambda_c D(\nabla C^n, \nabla\chi), \tag{1.15}$$

$$(\partial\Theta_1^n, \mu_1) + \lambda_1 L_1(\nabla\Theta_1^n, \nabla\mu_1) + L_1\Big(\partial_{\theta_1}\mathcal{F}(C^n, \Theta_1^n, \Theta_2^n), \mu_1\Big) = 0, \tag{1.16}$$

$$(\partial\Theta_2^n, \mu_2) + \lambda_2 L_2(\nabla\Theta_2^n, \nabla\mu_2) + L_2\Big(\partial_{\theta_2}\mathcal{F}(C^n, \Theta_1^n, \Theta_2^n), \mu_2\Big) = 0, \tag{1.17}$$

with $C^0 = c_0^h$, where c_0^h is some approximation of c_0 in S^h, $\Theta_1^0 = \theta_{10}^h$ and $\Theta_2^0 = \theta_{20}^h$, where θ_{i0}^h is some approximation of θ_{i0} in S^h, and

$$\partial Z^n = \frac{Z^n - Z^{n-1}}{k}$$

for a given sequence $\{Z^n\}_{n=0}^N$.

In the proof of existence of solutions, we use the discrete Green's operator $G^h : S_0^h \longrightarrow S_0^h$ defined by

$$(\nabla G^h v, \nabla\chi) = (v, \chi) \qquad \forall\chi \in S^h, \tag{1.18}$$

where $S_0^h = \{\chi \in S^h,\ (\chi, 1) = 0\}$.

Writing $|\chi|_{-h}^2 = |G^h\chi|_1^2$, it follows from (1.18) that

$$|\chi|_{-h}^2 = (G^h\chi, \chi) = (\chi, G^h\chi). \tag{1.19}$$

Throughout this section, we suppose that

$$k < \min\left\{\frac{4\lambda_c}{D(A + 4\gamma G_1)^2}, \frac{1}{2\overline{L}[\gamma G_2 + \overline{\varepsilon}(F_1 + F_2)]}\right\}, \tag{1.20}$$

with $\overline{\varepsilon} = \max\{\varepsilon_{12}, \varepsilon_{21}\}$ and $\overline{L} = \max\{L_1, L_2\}$.

Concerning Problem (1.14)–(1.17), we have the following result:

Theorem 1.2 Suppose that $c_0^h, \theta_{10}^h, \theta_{20}^h \in S^h$. Then there exists a unique solution $\{C^n, W^n, \Theta_1^n, \Theta_2^n\}$ to (1.14)–(1.17).

Proof. **Uniqueness**. Let $\{C_1^n, W_1^n, \Theta_{11}^n, \Theta_{21}^n\}$ and $\{C_2^n, W_2^n, \Theta_{12}^n, \Theta_{22}^n\}$ be two solutions of (1.14)–(1.17) and set $z^c = C_1^n - C_2^n$, $z^w = W_1^n - W_2^n$ and $z^{\theta_i} = \Theta_{i1}^n - \Theta_{i2}^n$. We start, stating the result when $n = 1$. Since $C_1^0 = C_2^0 = c_0^h$ and $\Theta_{i1}^0 = \Theta_{i2}^0 = \theta_0^h$, $i = 1, 2$, it follows from (1.14)–(1.17) that z^c, z^w, z^{θ_1} and z^{θ_2} satisfy

$$(z^c, \chi) + k(\nabla z^w, \nabla \chi) = 0, \tag{1.21}$$

$$\frac{1}{D}(z^w, \chi) = \Big(\partial_c \mathcal{F}(C_1^n, \Theta_{11}^n, \Theta_{21}^n) - \partial_c \mathcal{F}(C_2^n, \Theta_{12}^n, \Theta_{22}^n), \chi\Big) + \lambda_c(\nabla z^c, \nabla \chi), \tag{1.22}$$

$$\frac{1}{kL_1}(z^{\theta_1}, \mu_1) + \lambda_1(\nabla z^{\theta_1}, \nabla \mu_1) + \Big(\partial_{\theta_1} \mathcal{F}(C_1^n, \Theta_{11}^n, \Theta_{21}^n) - \partial_{\theta_1} \mathcal{F}(C_2^n, \Theta_{12}^n, \Theta_{22}^n), \mu_1\Big) = 0, \tag{1.23}$$

$$\frac{1}{kL_2}(z^{\theta_2}, \mu_2) + \lambda_2(\nabla z^{\theta_2}, \nabla \mu_2) + \Big(\partial_{\theta_2} \mathcal{F}(C_1^n, \Theta_{11}^n, \Theta_{21}^n) - \partial_{\theta_2} \mathcal{F}(C_2^n, \Theta_{12}^n, \Theta_{22}^n), \mu_2\Big) = 0. \tag{1.24}$$

Taking $\chi = z^w$ in (1.21) and $\chi = z^c$ in (1.22), subtracting the resulting equations and taking $\mu_i = z^{\theta_i}$ in (1.23)–(1.24), we obtain

$$\frac{k}{D}|z^w|_1^2 + \lambda_c|z^c|_1^2 = -\Big(\partial_c \mathcal{F}(C_1^n, \Theta_{11}^n, \Theta_{21}^n) - \partial_c \mathcal{F}(C_2^n, \Theta_{12}^n, \Theta_{22}^n), z^c\Big), \tag{1.25}$$

$$\frac{1}{kL_1}|z^{\theta_1}|^2 + \lambda_1|z^{\theta_1}|_1^2 = -\Big(\partial_{\theta_1} \mathcal{F}(C_1^n, \Theta_{11}^n, \Theta_{21}^n) - \partial_{\theta_1} \mathcal{F}(C_2^n, \Theta_{12}^n, \Theta_{22}^n), z^{\theta_1}\Big) \tag{1.26}$$

and

$$\frac{1}{kL_2}|z^{\theta_2}|^2 + \lambda_2|z^{\theta_2}|_1^2 = -\Big(\partial_{\theta_2} \mathcal{F}(C_1^n, \Theta_{11}^n, \Theta_{21}^n) - \partial_{\theta_2} \mathcal{F}(C_2^n, \Theta_{12}^n, \Theta_{22}^n), z^{\theta_2}\Big). \tag{1.27}$$

Writing

$$\phi(c) = -A(c - c_m) + B(c - c_m)^3 + D_\alpha(c - c_\alpha)^3 + D_\beta(c - c_\beta)^3 \qquad \text{and} \qquad \psi(\theta_i) = \delta\theta_i^3,$$

we have

$$(\partial_c \mathcal{F}(C_1^n, \Theta_{11}^n, \Theta_{21}^n) - \partial_c \mathcal{F}(C_2^n, \Theta_{12}^n, \Theta_{22}^n), z) = (\phi(C_1^n) - \phi(C_2^n), z)$$
$$- \gamma\Big(\partial_c g(C_1^n, \Theta_{11}^n) + \partial_c g(C_1^n, \Theta_{21}^n) - \partial_c g(C_2^n, \Theta_{12}^n) - \partial_c g(C_2^n, \Theta_{22}^n), z\Big),$$

$$\Big(\partial_{\theta_1} \mathcal{F}(C_1^n, \Theta_{11}^n, \Theta_{21}^n) - \partial_{\theta_1} \mathcal{F}(C_2^n, \Theta_{12}^n, \Theta_{22}^n), z\Big)$$
$$= \Big(\psi(\Theta_{11}^n) - \psi(\Theta_{12}^n) - \gamma[\partial_{\theta_1} g(C_1^n, \Theta_{11}^n) - \partial_{\theta_1} g(C_2^n, \Theta_{12}^n)], z\Big)$$
$$+ \Big(\varepsilon_{12}[\partial_u f(\Theta_{11}^n, \Theta_{21}^n) - \partial_u f(\Theta_{12}^n, \Theta_{22}^n)] + \varepsilon_{21}[\partial_v f(\Theta_{21}^n, \Theta_{11}^n) - \partial_v f(\Theta_{22}^n, \Theta_{12}^n)], z\Big)$$

and

$$\Big(\partial_{\theta_2} \mathcal{F}(C_1^n, \Theta_{11}^n, \Theta_{21}^n) - \partial_{\theta_2} \mathcal{F}(C_2^n, \Theta_{12}^n, \Theta_{22}^n), z\Big)$$
$$= \Big(\psi(\Theta_{21}^n) - \psi(\Theta_{22}^n) - \gamma[\partial_{\theta_2} g(C_1^n, \Theta_{21}^n) - \partial_{\theta_2} g(C_2^n, \Theta_{22}^n)], z\Big)$$
$$+ \Big(\varepsilon_{12}[\partial_v f(\Theta_{11}^n, \Theta_{21}^n) - \partial_v f(\Theta_{12}^n, \Theta_{22}^n)] + \varepsilon_{21}[\partial_u f(\Theta_{21}^n, \Theta_{11}^n) - \partial_u f(\Theta_{22}^n, \Theta_{12}^n)], z\Big).$$

From the Mean Value Theorem, there exists $\widetilde{C}$ such that

$$\Big(\phi(C_1^n) - \phi(C_2^n), z\Big) = \left(\frac{d\phi}{dc}(\widetilde{C})(C_1^n - C_2^n), z\right) = \left(\frac{d\phi}{dc}(\widetilde{C})z^c, z\right).$$

Hence,

$$-(\phi(C_1^n) - \phi(C_2^n), z^c) = -\Big(3[B(\widetilde{C} - c_m)^2 + D_\alpha(\widetilde{C} - c_\alpha)^2 + D_\beta(\widetilde{C} - c_\beta)^2]z^c, z^c\Big)$$
$$+ A(z^c, z^c) \leq A|z^c|^2.$$

In the same way, there exist $\widetilde{\Theta}_1$ and $\widetilde{\Theta}_2$, such that

$$-\Big(\psi(\Theta_{i1}^n) - \psi(\Theta_{i2}^n), z^{\theta_i}\Big) = -\Big(3\delta\widetilde{\Theta}_i^2(\Theta_{i1}^n - \Theta_{i2}^n), z^{\theta_i}\Big) \leq 0, \quad i = 1, 2.$$

Therefore, (1.25)–(1.27) become

$$\frac{k}{D}|z^w|_1^2 + \lambda_c|z^c|_1^2 \leq A|z^c|^2 + \gamma\sum_{i=1}^{2}\Big(\partial_c g(C_1^n, \Theta_{i1}^n) - \partial_c g(C_2^n, \Theta_{i2}^n), z^c\Big), \tag{1.28}$$

$$\frac{1}{kL_1}|z^{\theta_1}|^2 + \lambda_1 |z^{\theta_1}|_1^2 \le \gamma\Big(\partial_{\theta_1} g(C_1^n, \Theta_{11}^n) - \partial_{\theta_1} g(C_2^n, \Theta_{12}^n), z^{\theta_1}\Big)$$
$$- \Big(\varepsilon_{12}[\partial_u f(\Theta_{11}^n, \Theta_{21}^n) - \partial_u f(\Theta_{12}^n, \Theta_{22}^n)], z^{\theta_1}\Big)$$
$$- \Big(\varepsilon_{21}[\partial_v f(\Theta_{21}^n, \Theta_{11}^n) - \partial_v f(\Theta_{22}^n, \Theta_{12}^n)], z^{\theta_1}\Big)$$

and

$$\frac{1}{kL_2}|z^{\theta_2}|^2 + \lambda_2 |z^{\theta_2}|_1^2 \le \gamma\Big(\partial_{\theta_2} g(C_1^n, \Theta_{21}^n) - \partial_{\theta_2} g(C_2^n, \Theta_{22}^n), z^{\theta_2}\Big)$$
$$- \Big(\varepsilon_{12}[\partial_v f(\Theta_{11}^n, \Theta_{21}^n) - \partial_v f(\Theta_{12}^n, \Theta_{22}^n)], z^{\theta_2}\Big)$$
$$- \Big(\varepsilon_{21}[\partial_u f(\Theta_{21}^n, \Theta_{11}^n) - \partial_u f(\Theta_{22}^n, \Theta_{12}^n)], z^{\theta_2}\Big).$$

By adding the last two equations, we are left with

$$\frac{1}{kL_1}|z^{\theta_1}|^2 + \frac{1}{kL_2}|z^{\theta_2}|^2 + \lambda_1 |z^{\theta_1}|_1^2 + \lambda_2 |z^{\theta_2}|_1^2$$
$$\le \gamma \sum_{i=1}^{2} \Big([\partial_{\theta_i} g(C_1^n, \Theta_{i1}^n) - \partial_{\theta_i} g(C_2^n, \Theta_{i2}^n)] z^{\theta_i}, 1\Big)$$
$$- \varepsilon_{12}\Big([\nabla f(\Theta_{11}^n, \Theta_{21}^n) - \nabla f(\Theta_{12}^n, \Theta_{22}^n)] \cdot (z^{\theta_1}, z^{\theta_2}), 1\Big)$$
$$- \varepsilon_{21}\Big([\nabla f(\Theta_{21}^n, \Theta_{11}^n) - \nabla f(\Theta_{22}^n, \Theta_{12}^n)] \cdot (z^{\theta_2}, z^{\theta_1}), 1\Big).$$

By adding (1.28) and the last equation and using (1.9) and (1.10), we obtain

$$\frac{k}{D}|z^w|_1^2 + \lambda_c |z^c|_1^2 + \frac{1}{kL_1}|z^{\theta_1}|^2 + \frac{1}{kL_2}|z^{\theta_2}|^2 + \lambda_1 |z^{\theta_1}|_1^2 + \lambda_2 |z^{\theta_2}|_1^2$$
$$\le A|z^c|^2 + 2\gamma \sum_{i=1}^{2} [G_1 |z^c|^2 + G_2 |z^{\theta_i}|^2]$$
$$+ 2\varepsilon_{12}[F_1 |z^{\theta_1}|^2 + F_2 |z^{\theta_2}|^2] + 2\varepsilon_{21}[F_1 |z^{\theta_2}|^2 + F_2 |z^{\theta_1}|^2],$$

which by writing $\overline{\varepsilon} = \max\{\varepsilon_{12}, \varepsilon_{21}\}$, furnishes

$$\frac{k}{D}|z^w|_1^2 + \lambda_c |z^c|_1^2 + \frac{1}{kL_1}|z^{\theta_1}|^2 + \frac{1}{kL_2}|z^{\theta_2}|^2 + \lambda_1 |z^{\theta_1}|_1^2 + \lambda_2 |z^{\theta_2}|_1^2$$
$$\le [A + 4\gamma G_1]|z^c|^2 + \sum_{i=1}^{2} 2[\gamma G_2 + \overline{\varepsilon}(F_1 + F_2)]|z^{\theta_i}|^2.$$

By taking $\chi = z^c$ in (1.21) and using Hölder's and Young's inequalities, it results

$$\frac{k}{D}|z^w|_1^2 + \lambda_c|z^c|_1^2 + \frac{1}{kL_1}|z^{\theta_1}|^2 + \frac{1}{kL_2}|z^{\theta_2}|^2 + \lambda_1|z^{\theta_1}|_1^2 + \lambda_2|z^{\theta_2}|_1^2$$
$$\leq \frac{k}{D}|z^w|_1^2 + \frac{kD[A+4\gamma G_1]^2}{4}|z^c|_1^2 + \sum_{i=1}^{2} 2[\gamma G_2 + \bar{\varepsilon}(F_1+F_2)]|z^{\theta_i}|^2.$$

Therefore,

$$\left[\lambda_c - \frac{kD[A+4\gamma G_1]^2}{4}\right]|z^c|_1^2 + \sum_{i=1}^{2}\left[\frac{1}{kL_i} - 2[\gamma G_2 + \bar{\varepsilon}(F_1+F_2)]\right]|z^{\theta_i}|^2 \leq 0.$$

Since our assumptions on k imply that $\lambda_c - \frac{kD(A+4\gamma G_1)^2}{4} > 0$ and $\frac{1}{kL_i} - 2[\gamma G_2 + \bar{\varepsilon}(F_1 + F_2)] > 0$, we finally obtain

$$|z^c|_1^2 + |z^{\theta_1}|^2 + |z^{\theta_2}|^2 \leq 0.$$

Moreover, since $(z^c, 1) = 0$, Poincaré inequality implies that $|z^c| = 0$, and (1.22) now implies that $|z^w| = 0$. By induction on n, we conclude the proof of uniqueness.

Existence. As in Copetti & Elliott (1992), the existence of a solution of (1.14)–(1.17) for each $n = 1, \dots, N$ will be obtained by considering a minimization problem. In our case, such problem is to find $(C, \Theta_1, \Theta_2) \in K^h \times S^h \times S^h$ such that

$$\mathcal{F}^h(C, \Theta_1, \Theta_2) = \min_{(\chi,\mu_1,\mu_2)\in K^h\times S^h\times S^h} \mathcal{F}^h(\chi, \mu_1, \mu_2), \qquad (1.29)$$

where $K^h = \{\chi \in S^h,\ (\chi, 1) = (c_0^h, 1)\}$, S^h as before and

$$\mathcal{F}^h(\chi, \mu_1, \mu_2) = (\mathcal{F}(\chi, \mu_1, \mu_2), 1) + \frac{\lambda_c}{2}|\chi|_1^2 + \frac{1}{2Dk}|\chi - C^{n-1}|_{-h}^2$$
$$+ \frac{\lambda_1}{2}|\mu_1|_1^2 + \frac{\lambda_2}{2}|\mu_2|_1^2 + \frac{1}{2kL_1}|\mu_1 - \Theta_1^{n-1}|^2 + \frac{1}{2kL_2}|\mu_2 - \Theta_2^{n-1}|^2.$$

with $\mathcal{F}$ as in (1.8) and $|\cdot|_{-h}$ as defined in (1.19).

It follows from (1.9) and (1.10) that exists $m_{\mathcal{F}} \in R$ such that $\mathcal{F}(c, \theta_1, \theta_2) \geq m_{\mathcal{F}}$. Thus, from the definition of $\mathcal{F}^h$, we conclude that $\mathcal{F}^h$ is bounded below in $K^h \times S^h \times S^h$:

$$\mathcal{F}^h(\chi, \mu_1, \mu_2) \geq m_{\mathcal{F}}|\Omega| + \frac{\lambda_c}{2}|\chi|_1^2 + \sum_{i=1}^{2}\frac{1}{2kL_i}|\mu_i - \Theta_i^{n-1}|^2 \geq m_{\mathcal{F}}|\Omega|.$$

Let $d = \inf_{K^h\times S^h\times S^h} \mathcal{F}^h(\chi,\mu_1,\mu_2)$ and $\{\chi_m,\mu_{1m},\mu_{2m}\}$ be a minimizing sequence of $\mathcal{F}^h$ in $K^h\times S^h\times S^h$, that is the limit of $\mathcal{F}^h(\chi_m,\mu_{1m},\mu_{2m})$ when m goes to infinity is equal to d. It results from the above estimate and the Poincaré inequality that $\{\chi_m,\mu_{1m},\mu_{2m}\}$ is bounded in $L^2(\Omega)\times L^2(\Omega)\times L^2(\Omega)$. As a consequence, recalling that $K^h\times S^h\times S^h$ is finite dimensional, there exists $(C,\Theta_1,\Theta_2)\in S^h\times S^h\times S^h$ and a subsequence $\{\chi_m,\mu_{1m},\mu_{2m}\}$ such that

$$\chi_m \text{ converges to } C \qquad \text{and} \qquad \mu_{im} \text{ converges to } \Theta_i \qquad \text{in} \qquad S^h.$$

Since K^h is closed, $C\in K^h$ and the continuity of $\mathcal{F}^h$ in $S^h\times S^h\times S^h$ yields that $\mathcal{F}^h(\chi_m,\mu_{1m},\mu_{2m})$ converges to $\mathcal{F}^h(C,\Theta_1,\Theta_2)$ and also to d. Therefore, there exists a solution (C,Θ_1,Θ_2) to (1.29). By the standard arguments of calculus of variations, the minimizer (C,Θ_1,Θ_2) satisfies: $\forall(\chi,\mu_1,\mu_2)\in S^h\times S^h\times S^h$,

$$\lambda_c(\nabla C,\nabla\chi) + \Big(\partial_c\mathcal{F}(C,\Theta_1,\Theta_2),\chi\Big) + \frac{1}{D}\left(G^h\left(\frac{C-C^{n-1}}{k}\right),\chi\right) - \lambda(1,\chi) = 0,$$

$$\lambda_1(\nabla\Theta_1,\nabla\mu_1) + \Big(\partial_{\theta_1}\mathcal{F}(C,\Theta_1,\Theta_2),\mu_1\Big) + \frac{1}{L_1}\left(\frac{\Theta_1-\Theta_1^{n-1}}{k},\mu_1\right) = 0,$$

$$\lambda_2(\nabla\Theta_2,\nabla\mu_2) + \Big(\partial_{\theta_2}\mathcal{F}(C,\Theta_1,\Theta_2),\mu_2\Big) + \frac{1}{L_2}\left(\frac{\Theta_2-\Theta_2^{n-1}}{k},\mu_2\right) = 0,$$

where $\lambda = \frac{1}{|\Omega|}\Big(\partial_c\mathcal{F}(C,\Theta_1,\Theta_2),1\Big)$ is a Lagrange multiplier, and G^h is the discrete Green's operator defined in (1.18). By defining

$$C^n = C,\quad W^n = \lambda D - G^h(\partial C^n),\quad \Theta_1^n = \Theta_1 \quad\text{and}\quad \Theta_2^n = \Theta_2,$$

it follows that $\{C^n,W^n,\Theta_1^n,\Theta_2^n\}$ is a solution of (1.14)–(1.17). ■

Now, we proceed to obtain a priori estimates for the previous approximate solutions. We start with the following Lemma:

LEMMA 1.1 The following stability estimates hold

$$k\sum_{r=1}^{n}|W^r|_1^2 + k^2\sum_{r=1}^{n}|\partial C^r|_1^2 + |C^n|_1^2 \le C. \tag{1.30}$$

and

$$k\sum_{r=1}^{n}\sum_{i=1}^{2}|\partial\Theta_i^r|^2 + k^2\sum_{r=1}^{n}\sum_{i=1}^{2}|\partial\Theta_i^r|_1^2 + \sum_{i=1}^{2}|\Theta_i^n| + \sum_{i=1}^{2}|\Theta_i^n|_1^2 \le C. \tag{1.31}$$

Proof. Choosing $\chi = W^n$ in (1.14), $\chi = \partial C^n$ in (1.15) and $\mu_i = \partial\Theta_i^n$ in (1.16)–(1.17), we obtain

$$\frac{1}{D}|W^n|_1^2 = -\frac{1}{D}\Big(\partial C^n, W^n\Big) = -\Big(\partial_c\mathcal{F}(C^n,\Theta_1^n,\Theta_2^n),\partial C^n\Big) - \lambda_c\Big(\nabla C^n, \nabla[\partial C^n]\Big),$$
$$\frac{1}{L_1}|\partial\Theta_1^n|^2 + \lambda_1\Big(\nabla\Theta_1^n, \nabla[\partial\Theta_1^n]\Big) = -\Big(\partial_{\theta_1}\mathcal{F}(C^n,\Theta_1^n,\Theta_2^n),\partial\Theta_1^n\Big)$$

and

$$\frac{1}{L_2}|\partial\Theta_2^n|^2 + \lambda_2\Big(\nabla\Theta_2^n, \nabla[\partial\Theta_2^n]\Big) = -\Big(\partial_{\theta_2}\mathcal{F}(C^n,\Theta_1^n,\Theta_2^n),\partial\Theta_2^n\Big).$$

Hence, summing the above equations, we obtain

$$\begin{aligned}\frac{1}{D}|W^n|_1^2 + \lambda_c\Big(\nabla C^n, \nabla[\partial C^n]\Big) + \sum_{i=1}^{2}\left[\frac{1}{L_i}|\partial\Theta_i^n|^2 + \lambda_i(\nabla\Theta_i^n, \nabla[\partial\Theta_i^n])\right] \\ = -\nabla\mathcal{F}(C^n,\Theta_1^n,\Theta_2^n)\cdot(\partial C^n, \partial\Theta_1^n, \partial\Theta_2^n).\end{aligned} \tag{1.32}$$

To estimate the terms at the right-hand side, let us note that the function $[\mathcal{F}+H](C^n,\Theta_1^n,\Theta_2^n)$ is convex, where

$$H(C^n,\Theta_1^n,\Theta_2^n) = \frac{A}{2}(C^n - c_m)^2 + \gamma\sum_{i=1}^{2} g(C^n,\Theta_i^n) - \sum_{i=1}^{2}\sum_{i\neq j=1}^{2}\varepsilon_{ij} f(\Theta_i^n,\Theta_j^n).$$

We also observe that

$$\begin{aligned}&\nabla H(C^n,\Theta_1^n,\Theta_2^n)\cdot(\partial C^n,\partial\Theta_1^n,\partial\Theta_2^n)\\ &\qquad = A(C^n - c_m)\partial C^n + \gamma\sum_{i=1}^{2}\nabla g(C^n,\Theta_i^n)\cdot(\partial C^n,\partial\Theta_i^n)\\ &\qquad - \varepsilon_{12}\nabla f(\Theta_1^n,\Theta_2^n)\cdot(\partial\Theta_1^n,\partial\Theta_2^n) - \varepsilon_{21}\nabla f(\Theta_2^n,\Theta_1^n)\cdot(\partial\Theta_2^n,\partial\Theta_1^n).\end{aligned}$$

Thus, by using the convexity of $\mathcal{F} + H$, we obtain

$$
\begin{aligned}
-\frac{1}{k}\nabla\mathcal{F}(C^n, \Theta_1^n, \Theta_2^n) &\cdot (C^n - C^{n-1}, \Theta_1^n - \Theta_1^{n-1}, \Theta_2^n - \Theta_2^{n-1}) \\
&\leq \frac{1}{k}[\mathcal{F}(C^{n-1}, \Theta_1^{n-1}, \Theta_2^{n-1}) + H(C^{n-1}, \Theta_1^{n-1}, \Theta_2^{n-1})] \\
&- \frac{1}{k}[\mathcal{F}(C^n, \Theta_1^n, \Theta_2^n) - H(C^n, \Theta_1^n, \Theta_2^n)] \\
&+ \nabla H(C^n, \Theta_1^n, \Theta_2^n) \cdot (\partial C^n, \partial\Theta_1^n, \partial\Theta_2^n) \\
&= \frac{1}{k}[\mathcal{F}(C^{n-1}, \Theta_1^{n-1}, \Theta_2^{n-1}) - \mathcal{F}(C^n, \Theta_1^n, \Theta_2^n)] \\
&+ \frac{A}{2k}(C^{n-1} - c_m)^2 - \frac{A}{2k}(C^n - c_m)^2 + A(C^n - c_m)\partial C^n \\
&+ \gamma\sum_{i=1}^{2}\left[\frac{1}{k}[g(C^{n-1}, \Theta_i^{n-1}) - g(C^n, \Theta_i^n)] + \nabla g(C^n, \Theta_i^n) \cdot (\partial C^n, \partial\Theta_i^n)\right] \\
&- \varepsilon_{12}\left[\frac{1}{k}[f(\Theta_1^{n-1}, \Theta_2^{n-1}) - f(\Theta_1^n, \Theta_2^n)] + \nabla f(\Theta_1^n, \Theta_2^n) \cdot (\partial\Theta_1^n, \partial\Theta_2^n)\right] \\
&- \varepsilon_{21}\left[\frac{1}{k}[f(\Theta_2^{n-1}, \Theta_1^{n-1}) - f(\Theta_2^n, \Theta_1^n)] + \nabla f(\Theta_2^n, \Theta_1^n) \cdot (\partial\Theta_2^n, \partial\Theta_1^n)\right].
\end{aligned}
$$

Now, by using (1.9) and (1.10)

$$
\begin{aligned}
-\nabla\mathcal{F}&(C^n, \Theta_1^n, \Theta_2^n) \cdot (\partial C^n, \partial\Theta_1^n, \partial\Theta_2^n) \\
&\leq \frac{1}{k}[\mathcal{F}(C^{n-1}, \Theta_1^{n-1}, \Theta_2^{n-1}) - \mathcal{F}(C^n, \Theta_1^n, \Theta_2^n)] + \frac{A}{2k}(C^{n-1} - C^n)(C^{n-1} - C^n) \\
&\quad + 2k\gamma G_1(\partial C^n)^2 + k\sum_{i=1}^{2}\Big[\gamma G_2 + \overline{\varepsilon}(F_1 + F_2)\Big](\partial\Theta_i^n)^2 \\
&= \frac{1}{k}[\mathcal{F}(C^{n-1}, \Theta_1^{n-1}, \Theta_2^{n-1}) - \mathcal{F}(C^n, \Theta_1^n, \Theta_2^n)] + \frac{k(A + 4\gamma G_1)}{2}(\partial C^n)^2 \\
&\quad + k\sum_{i=1}^{2}\Big[\gamma G_2 + \overline{\varepsilon}(F_1 + F_2)\Big](\partial\Theta_i^n)^2.
\end{aligned}
$$

Let us note that

$$
(\nabla C^n, \nabla[\partial C^n]) = \frac{[|C^n|_1^2 - |C^{n-1}|_1^2]}{2k} + \frac{k}{2}|\partial C^n|_1^2 = \frac{1}{2}\partial[|C^n|_1^2] + \frac{k}{2}|\partial C^n|_1^2.
$$

Therefore, (1.32) becomes

$$\frac{k}{D}|W^n|_1^2 + \frac{k^2\lambda_c}{2}|\partial C^n|_1^2 + \frac{k\lambda_c}{2}\partial[|C^n|_1^2] + \sum_{i=1}^{2}\frac{k\lambda_i}{2}\left[\frac{2}{\lambda_i L_i}|\partial\Theta_i^n|^2 + k|\partial\Theta_i^n|_1^2 + \partial[|\Theta_i^n|_1^2]\right]$$
$$\leq \Big(\mathcal{F}(C^{n-1},\Theta_1^{n-1},\Theta_2^{n-1}) - \mathcal{F}(C^n,\Theta_1^n,\Theta_2^n),1\Big)$$
$$+\frac{k^2(A+4\gamma G_1)}{2}|\partial C^n|^2 + k^2\sum_{i=1}^{2}[\gamma G_2 + \bar{\varepsilon}(F_1+F_2)]|\partial\Theta_i^n|^2.$$

Now, the term having $|\partial C^n|^2$ can be estimated by taking $\chi = \partial C^n$ in (1.14). We obtain

$$|\partial C^n|^2 = -\Big(\nabla W^n, \nabla\partial C^n\Big) \leq \frac{1}{kD(A+4\gamma G_1)}|W^n|_1^2 + \frac{kD(A+4\gamma G_1)}{4}|\partial C^n|_1^2,$$

and therefore,

$$\frac{k}{2D}|W^n|_1^2 + \frac{k^2\lambda_c}{2}|\partial C^n|_1^2 + \frac{k\lambda_c}{2}\partial[|C^n|_1^2] + \sum_{i=1}^{2}\frac{k\lambda_i}{2}\left[\frac{2}{\lambda_i L_i}|\partial\Theta_i^n|^2 + k|\partial\Theta_i^n|_1^2 + \partial[|\Theta_i^n|_1^2]\right]$$
$$\leq \Big(\mathcal{F}(C^{n-1},\Theta_1^{n-1},\Theta_2^{n-1}) - \mathcal{F}(C^n,\Theta_1^n,\Theta_2^n),1\Big)$$
$$+k^2\left[\frac{kD(A+4\gamma G_1)^2}{8}\right]|\partial C^n|_1^2 + k^2\sum_{i=1}^{2}[\gamma G_2 + \bar{\varepsilon}(F_1+F_2)]|\partial\Theta_i^n|^2.$$

That is,

$$\frac{k}{2D}|W^n|_1^2 + \frac{k^2}{2}\left[\lambda_c - \frac{kD(A+4\gamma G_1)^2}{4}\right]|\partial C^n|_1^2 + \frac{k\lambda_c}{2}\partial[|C^n|_1^2]$$
$$+k\sum_{i=1}^{2}\left[\frac{1-kL_i[\gamma G_2 + \bar{\varepsilon}(F_1+F_2)]}{L_i}\right]|\partial\Theta_i^n|^2 + \sum_{i=1}^{2}\left[\frac{k^2\lambda_i}{2}|\partial\Theta_i^n|_1^2 + \frac{k\lambda_i}{2}\partial[|\Theta_i^n|_1^2]\right]$$
$$\leq (\mathcal{F}(C^{n-1},\Theta_1^{n-1},\Theta_2^{n-1}) - \mathcal{F}(C^n,\Theta_1^n,\Theta_2^n),1).$$

By summing over n, it results that

$$\frac{k}{2D}\sum_{r=1}^{n}|W^r|_1^2+\frac{k^2}{2}\left[\lambda_c-\frac{kD(A+4\gamma G_1)^2}{4}\right]\sum_{r=1}^{n}|\partial C^r|_1^2+\frac{\lambda_c}{2}|C^n|_1^2+\sum_{i=1}^{2}\frac{\lambda_i}{2}|\Theta_i^n|_1^2$$
$$+k\sum_{r=1}^{n}\sum_{i=1}^{2}\left[\frac{1-kL_i[\gamma G_2+\bar{\varepsilon}(F_1+F_2)]}{L_i}\right]|\partial\Theta_i^r|^2+\sum_{r=1}^{n}\sum_{i=1}^{2}\frac{k^2\lambda_i}{2}|\partial\Theta_i^r|_1^2$$
$$+(\mathcal{F}(C^n,\Theta_1^n,\Theta_2^n),1)\leq(\mathcal{F}(C^0,\Theta_1^0,\Theta_2^0),1)+\frac{\lambda_c}{2}|C^0|_1^2+\sum_{i=1}^{2}\frac{\lambda_i}{2}|\Theta_i^0|_1^2\leq C(c_0^h,\theta_{10}^h,\theta_{20}^h),$$

and (1.30) is proved since we have (1.20) and $\mathcal{F}$ is bounded below.

The above inequality gives an estimate to $(\mathcal{F}(C^n,\Theta_1^n,\Theta_2^n),1)$. Using such estimate, (1.30) and the Poincaré inequality, we obtain

$$|\Theta_1^n|+|\Theta_2^n|\leq C$$

and (1.31) is proved. ■

We also have:

LEMMA 1.2 For $t_n>0$, where $t_n=nk$, there holds

$$t_n|W^n|_1^2+k\sum_{r=1}^{n}t_r|\partial C^r|_1^2+\sum_{i=1}^{2}t_n|\partial\Theta_i^n|^2+k\sum_{r=1}^{n}\sum_{i=1}^{2}t_r|\partial\Theta_i^r|_1^2\leq C. \tag{1.33}$$

Proof. From equation (1.15), we have

$$(\partial W^n,\chi)=D\Big(\partial\Big[\partial_c\mathcal{F}(C^n,\Theta_1^n,\Theta_2^n)\Big],\chi\Big)+\lambda_c D(\nabla\partial C^n,\nabla\chi).$$

By taking $\chi=\partial C^n$ in the above equation and $\chi=\partial W^n$ in (1.14), it results

$$-(\nabla W^n,\nabla\partial W^n)=(\partial C^n,\partial W^n)=D\Big(\partial\Big[\partial_c\mathcal{F}(C^n,\Theta_1^n,\Theta_2^n)\Big],\partial C^n\Big)+\lambda_c D|\partial C^n|_1^2.$$

As it was noted before, we could rewrite the above equation as

$$\frac{1}{2D}\partial[|W^n|_1^2]+\frac{k}{2D}|\partial W^n|_1^2+\Big(\partial\Big[\partial_c\mathcal{F}(C^n,\Theta_1^n,\Theta_2^n)\Big],\partial C^n\Big)+\lambda_c|\partial C^n|_1^2=0.$$

By taking $\mu = \partial\Theta_i^n$ in (1.16)–(1.17), we obtain

$$\frac{1}{L_i}|\partial\Theta_i^n|^2 + \lambda_i\Big(\nabla\Theta_i^n, \nabla\Big[\partial\Theta_i^n\Big]\Big) + \Big(\partial_{\theta_i}\mathcal{F}(C^n, \Theta_1^n, \Theta_2^n), \partial\Theta_i^n\Big) = 0$$

and

$$\frac{1}{L_i}\Big(\partial\Theta_i^{n-1}, \partial\Theta_i^n\Big) + \lambda_i\Big(\nabla\Theta_i^{n-1}, \nabla\Big[\partial\Theta_i^n\Big]\Big) + \Big(\partial_{\theta_i}\mathcal{F}(C^{n-1}, \Theta_1^{n-1}, \Theta_2^{n-1}), \partial\Theta_i^n\Big) = 0.$$

By subtracting the above two equations, we obtain

$$\frac{1}{L_i}|\partial\Theta_i^n|^2 + k\lambda_i|\partial\Theta_i^n|_1^2 + k\Big(\partial\Big[\partial_{\theta_i}\mathcal{F}(C^n, \Theta_1^n, \Theta_2^n)\Big], \partial\Theta_i^n\Big) = \frac{1}{L_i}\Big(\partial\Theta_i^{n-1}, \partial\Theta_i^n\Big).$$

Dividing by k and using the Hölder's and Young's inequalities, it results

$$\frac{1}{2kL_1}[|\partial\Theta_1^n|^2 - |\partial\Theta_1^{n-1}|^2] + \lambda_1|\partial\Theta_1^n|_1^2 + \Big(\partial\Big[\partial_{\theta_1}\mathcal{F}(C^n, \Theta_1^n, \Theta_2^n)\Big], \partial\Theta_1^n\Big) \le 0$$

and

$$\frac{1}{2kL_2}[|\partial\Theta_2^n|^2 - |\partial\Theta_2^{n-1}|^2] + \lambda_2|\partial\Theta_2^n|_1^2 + \Big(\partial\Big[\partial_{\theta_2}\mathcal{F}(C^n, \Theta_1^n, \Theta_2^n)\Big], \partial\Theta_2^n\Big) \le 0.$$

Therefore,

$$\begin{aligned}\frac{1}{2D}\partial[|W^n|_1^2] + \frac{k}{2D}|\partial W^n|_1^2 + \lambda_c|\partial C^n|_1^2 + \sum_{i=1}^{2}\Big[\frac{1}{2L_i}\partial[|\partial\Theta_i^n|^2] + \lambda_i|\partial\Theta_i^n|_1^2\Big] \\ + \Big(\nabla[\partial\mathcal{F}(C^n, \Theta_1^n, \Theta_2^n)]\cdot(\partial C^n, \partial\Theta_1^n, \partial\Theta_2^n), 1\Big) \le 0.\end{aligned} \tag{1.34}$$

We note that if $h(r, s)$ is a convex function, we have

$$\nabla[h(r, s) - h(u, v)]\cdot(r - u, s - v) \ge 0.$$

Now we use a convexity argument similar to the one used in the last Lemma. Observe that the function $[\mathcal{F} + H](C^n, \Theta_1^n, \Theta_2^n)$ is convex, if we take

$$H(C^n, \Theta_1^n, \Theta_2^n) = \frac{A}{2}(C^n - c_m)^2 + \gamma\sum_{i=1}^{2} g(C^n, \Theta_i^n) - \sum_{i=1}^{2}\sum_{i\neq j=1}^{2}\varepsilon_{ij}f(\Theta_i^n, \Theta_j^n).$$

We also have

$$\nabla[\partial H(C^n,\Theta_1^n,\Theta_2^n)]\cdot(\partial C^n,\partial\Theta_1^n,\partial\Theta_2^n)=\frac{A}{k}[(C^n-c_m)-(C^{n-1}-c_m)]\partial C^n$$
$$+\frac{\gamma}{k}\sum_{i=1}^{2}\nabla[g(C^n,\Theta_i^n)-g(C^{n-1},\Theta_i^{n-1})]\cdot(\partial C^n,\partial\Theta_i^n)$$
$$-\frac{\varepsilon_{12}}{k}\nabla[f(\Theta_1^n,\Theta_2^n)-f(\Theta_1^{n-1},\Theta_2^{n-1})]\cdot(\partial\Theta_1^n,\partial\Theta_2^n)$$
$$-\frac{\varepsilon_{21}}{k}\nabla[f(\Theta_2^n,\Theta_1^n)-f(\Theta_2^{n-1},\Theta_1^{n-1})]\cdot(\partial\Theta_2^n,\partial\Theta_1^n).$$

Thus, since $\mathcal{F}+H$ is a convex function, we obtain

$$\nabla[\partial\mathcal{F}(C^n,\Theta_1^n,\Theta_2^n)]\cdot(\partial C^n,\partial\Theta_1^n,\partial\Theta_2^n)\geq-\nabla[\partial H(C^n,\Theta_1^n,\Theta_2^n)]\cdot(\partial C^n,\partial\Theta_1^n,\partial\Theta_2^n).$$

The above inequality and (1.34) imply that

$$\frac{1}{2D}\partial[|W^n|_1^2]+\frac{k}{2D}|\partial W^n|_1^2+\lambda_c|\partial C^n|_1^2+\sum_{i=1}^{2}\Big[\frac{1}{2L_i}\partial[|\partial\Theta_i^n|^2]+\lambda_i|\partial\Theta_i^n|_1^2\Big]$$
$$-(\nabla[\partial H(C^n,\Theta_1^n,\Theta_2^n)]\cdot(\partial C^n,\partial\Theta_1^n,\partial\Theta_2^n),1)\leq 0.$$

That is,

$$\frac{1}{2D}\partial[|W^n|_1^2]+\frac{k}{2D}|\partial W^n|_1^2+\lambda_c|\partial C^n|_1^2+\sum_{i=1}^{2}\frac{1}{2L_i}\partial[|\partial\Theta_i^n|^2]+\sum_{i=1}^{2}\lambda_i|\partial\Theta_i^n|_1^2$$
$$\leq A|\partial C^n|^2+\frac{\gamma}{k}\sum_{i=1}^{2}\Big(\nabla\Big[g(C^n,\Theta_i^n)-g(C^{n-1},\Theta_i^{n-1})\Big]\cdot(\partial C^n,\partial\Theta_i^n),1\Big)$$
$$-\frac{1}{k}\sum_{i=1}^{2}\sum_{i\neq j=1}^{2}\varepsilon_{ij}\Big(\nabla\Big[f(\Theta_i^n,\Theta_j^n)-f(\Theta_i^{n-1},\Theta_j^{n-1})\Big]\cdot(\partial\Theta_i^n,\partial\Theta_j^n),1\Big)$$

(from (1.9) and (1.10)),

$$\leq A|\partial C^n|^2+2\sum_{i=1}^{2}\left(\gamma[G_1(\partial C^n)^2+G_2(\partial\Theta_i^n)^2]+\sum_{i\neq j=1}^{2}\varepsilon_{ij}[F_1(\partial\Theta_i^n)^2+F_2(\partial\Theta_j^n)^2],1\right)$$
$$\leq(A+4\gamma G_1)|\partial C^n|^2+\sum_{i=1}^{2}2[\gamma G_2+\bar{\varepsilon}(F_1+F_2)]|\partial\Theta_i^n|^2.$$

From (1.14), we obtain

$$\frac{1}{2D}\partial[|W^n|_1^2] + \frac{k}{2D}|\partial W^n|_1^2 + \lambda_c|\partial C^n|_1^2 + \sum_{i=1}^{2}\frac{1}{2L_i}\partial[|\partial\Theta_i^n|^2] + \sum_{i=1}^{2}\lambda_i|\partial\Theta_i^n|_1^2$$
$$\leq -(A+4\gamma G_1)(\nabla W^n, \nabla\partial C^n) + \sum_{i=1}^{2}2[\gamma G_2 + \bar{\varepsilon}(F_1+F_2)]|\partial\Theta_i^n|^2$$
$$\leq \frac{(A+4\gamma G_1)^2}{2\lambda_c}|W^n|_1^2 + \frac{\lambda_c}{2}|\partial C^n|_1^2 + \sum_{i=1}^{2}2[\gamma G_2 + \bar{\varepsilon}(F_1+F_2)]|\partial\Theta_i^n|^2.$$

Multiplying the above inequality by $2k$ yields

$$\frac{1}{D}[|W^n|_1^2 - |W^{n-1}|_1^2] + k\lambda_c|\partial C^n|_1^2 + \sum_{i=1}^{2}\frac{1}{L_i}[|\partial\Theta_i^n|^2 - |\partial\Theta_i^{n-1}|^2] + 2k\sum_{i=1}^{2}\lambda_i|\partial\Theta_i^n|_1^2$$
$$\leq \frac{k(A+4\gamma G_1)^2}{\lambda_c}|W^n|_1^2 + k\sum_{i=1}^{2}4[\gamma G_2 + \bar{\varepsilon}(F_1+F_2)]|\partial\Theta_i^n|^2.$$

Now, by multiplying by $t_n = nk$, we obtain

$$\frac{1}{D}[t_n|W^n|_1^2 - t_{n-1}|W^{n-1}|_1^2] + kt_n\lambda_c|\partial C^n|_1^2 + \sum_{i=1}^{2}\frac{1}{L_i}[t_n|\partial\Theta_i^n|^2 - t_{n-1}|\partial\Theta_i^{n-1}|^2]$$
$$+ 2kt_n\sum_{i=1}^{2}\lambda_i|\partial\Theta_i^n|_1^2 \leq \frac{k}{D}|W^{n-1}|_1^2 + k\sum_{i=1}^{2}\frac{1}{L_i}|\partial\Theta_i^{n-1}|^2 + \frac{kT(A+4\gamma G_1)^2}{\lambda_c}|W^n|_1^2$$
$$+ kT\sum_{i=1}^{2}4[\gamma G_2 + \bar{\varepsilon}(F_1+F_2)]|\partial\Theta_i^n|^2.$$

By summing over n we obtain

$$\frac{t_n}{D}|W^n|_1^2 + k\lambda_c\sum_{r=2}^{n}t_r|\partial C^r|_1^2 + \sum_{i=1}^{2}\frac{t_n}{L_i}|\partial\Theta_i^n|^2 + 2k\sum_{r=2}^{n}\sum_{i=1}^{2}t_r\lambda_i|\partial\Theta_i^r|_1^2$$
$$\leq \frac{kT(A+4\gamma G_1)^2}{\lambda_c}\sum_{r=2}^{n}|W^r|_1^2 + kT\sum_{r=2}^{n}\sum_{i=1}^{2}4[\gamma G_2 + \bar{\varepsilon}(F_1+F_2)]|\partial\Theta_i^r|^2$$
$$+ \frac{k}{D}\sum_{r=2}^{n}|W^{r-1}|_1^2 + k\sum_{r=2}^{n}\sum_{i=1}^{2}\frac{1}{L_i}|\partial\Theta_i^{r-1}|^2 + \frac{t_1}{D}|W^1|_1^2 + \sum_{i=1}^{2}\frac{1}{L_i}t_1|\partial\Theta_i^1|^2.$$

From (1.30), with $n = 1$, and recalling that $t_1 = k$, it follows that

$$t_1|W^1|_1^2 + kt_1|\partial C^1|_1^2 + t_1\sum_{i=1}^{2}|\partial\Theta_i^1|^2 + 2kt_1\sum_{i=1}^{2}|\partial\Theta_i^1|_1^2 \le C.$$

Therefore, using Lemma 1.1, we conclude that

$$t_n|W^n|_1^2 + k\sum_{r=1}^{n} t_r|\partial C^r|_1^2 + \sum_{i=1}^{2} t_n|\partial\Theta_i^n|^2 + k\sum_{r=1}^{n}\sum_{i=1}^{2} t_r|\partial\Theta_i^r|_1^2 \le C.$$

∎

1.4 Convergence of the approximate solutions

In this section we pass to the limit in the sequence of approximate solutions. We start introducing the H^1-projection, $R^h : H^1(\Omega) \longrightarrow S^h$, defined by

$$(\nabla R^h v, \nabla\chi) = (\nabla v, \nabla\chi) \qquad \forall\chi \in S^h$$
$$(R^h v, 1) = (v, 1).$$

It holds that $R^h v$ converges to v in $H^1(\Omega)$ strongly and $|R^h v|_1 \le |v|_1$.

Given $c_0^h, \theta_{10}, \theta_{20} \in H^1(\Omega)$, let us take $c_0^h = P^h c_0$, $\theta_{10}^h = P^h\theta_{10}$ and $\theta_{20}^h = P^h\theta_{20}$, where $P^h w$ is the unique solution of

$$(P^h w, \chi) = (w, \chi), \qquad \forall\chi \in S^h.$$

Therefore c_0^h, θ_{10}^h and θ_{20}^h satisfy the assumptions of Theorem 1.2

For $t \in (t_{n-1}, t_n)$, $1 \le n \le N$, we define the following piecewise constant functions

$$\begin{aligned}
&c_k^h(t) = C^n, && w_k^h(t) = W^n,\\
&\theta_{1k}^h(t) = \Theta_1^n, && \theta_{2k}^h(t) = \Theta_2^n\\
&\mathcal{F}_{hk}^c(t) = \partial_c\mathcal{F}(C^n, \Theta_1^n, \Theta_2^n), &&\\
&\mathcal{F}_{hk}^{\theta_i}(t) = \partial_{\theta_i}\mathcal{F}(C^n, \Theta_1^n, \Theta_2^n), && \text{for} \quad i = 1, 2.
\end{aligned}$$

Analogously, for a given $\xi \in C^\infty(0, T)$, we define

$$\xi_k(t) = \xi(t_{n-1}) = \xi^{n-1} \quad \text{for } t \in (t_{n-1}, t_n),\ 1 \le n \le N.$$

We also denote by $\widehat{c}_k^h$, $\widehat{\theta}_{1k}^h, \widehat{\theta}_{2k}^h$ and $\widehat{\xi}_k$ the corresponding piecewise linear continuous functions on $[0, T]$ defined by

$$\begin{aligned}
&\widehat{c}_k^h(t_n) = C^n, \quad n = 0, \dots, N, \\
&\widehat{\theta}_{1k}^h(t_n) = \Theta_1^n, \quad n = 0, \dots, N, \\
&\widehat{\theta}_{2k}^h(t_n) = \Theta_2^n, \quad n = 0, \dots, N, \\
&\widehat{\xi}_k(t_n) = \xi^n, \quad n = 0, \dots, N-1, \\
&\widehat{\xi}_k(T) = \xi^{N-1}.
\end{aligned}$$

Now, the estimates given (1.30), (1.31) and (1.33) easily imply that

$$\begin{array}{lll}
c_k^h,\ \theta_{1k}^h,\ \theta_{2k}^h & \text{are uniformly bounded in} & L^\infty(0, T, H^1(\Omega)), \\
\widehat{c}_k^h,\ \widehat{\theta}_{1k}^h,\ \widehat{\theta}_{2k}^h & \text{are uniformly bounded in} & L^\infty(0, T, H^1(\Omega)), \\
\sqrt{t}\partial_t\widehat{c}_k^h,\ \sqrt{t}\partial_t\widehat{\theta}_{1k}^h,\ \sqrt{t}\partial_t\widehat{\theta}_{2k}^h & \text{are uniformly bounded in} & L^2(0, T, H^1(\Omega)).
\end{array}$$

Since we have the injection of $H^1(\Omega)$ into $L^6(\Omega)$, (1.9) and (1.10), it results

$$\mathcal{F}_{hk}^c,\ \mathcal{F}_{hk}^{\theta_1},\ \mathcal{F}_{hk}^{\theta_2} \qquad \text{are uniformly bounded in} \qquad L^\infty(0, T, L^2(\Omega)).$$

Now we prove that $\sqrt{t_n}W^n$ is uniformly bounded in $H^1(\Omega)$. From estimate in (1.33), to obtain this result, it is enough to show that

$$t_n|W^n|^2 \leq C.$$

For this, let us recall the definition of W^n:

$$W^n = \frac{D}{|\Omega|}\Big(\partial_c\mathcal{F}(C^n, \Theta_1^n, \Theta_2^n), 1\Big) - G^h(\partial C^n).$$

Now, to estimate the first term in the right hand side, we use the injection of $H^1(\Omega)$ into $L^6(\Omega)$ and (1.10) to obtain an uniform estimate of $\partial_c\mathcal{F}(C^n, \Theta_1^n, \Theta_2^n)$ in $L^2(\Omega)$. Since $G^h(\partial C^n)$ has zero mean value, we obtain from (1.33) that

$$t_n|W^n|^2 \leq C + t_nC|G^h(\partial C^n)|_1^2 \leq C + t_nC|W^n|_1^2 \leq C.$$

The obtained estimate for W^n, implies that

$$\sqrt{t}w_k^h \text{ is uniformly bounded in } L^\infty(0, T, H^1(\Omega)).$$

Therefore there exist $\{c, \widehat{c}, w, \mathcal{F}^c, \mathcal{F}^{\theta_1}, \mathcal{F}^{\theta_2}\}$, $\{\theta_1, \widehat{\theta}_1, \theta_2, \widehat{\theta}_2\}$ such that

$$c,\ \theta_1,\ \theta_2 \in L^\infty(0,T,H^1(\Omega)),$$
$$\widehat{c},\ \widehat{\theta}_1,\ \widehat{\theta}_2 \in L^\infty(0,T,H^1(\Omega)),$$
$$\sqrt{t}\partial_t\widehat{c},\ \sqrt{t}\partial_t\widehat{\theta}_1,\ \sqrt{t}\partial_t\widehat{\theta}_2 \in L^2(0,T,H^1(\Omega)),$$
$$\mathcal{F}^c,\ \mathcal{F}^{\theta_1},\ \mathcal{F}^{\theta_2} \in L^\infty(0,T,L^2(\Omega)),$$
$$\sqrt{t}w \in L^\infty(0,T,H^1(\Omega))$$

and subsequences $\{c_k^h, \widehat{c}_k^h, w_k^h, \mathcal{F}_{hk}^c\}$, $\{\mathcal{F}_{hk}^{\theta_i}, \theta_{ik}^h, \widehat{\theta}_{ik}^h\}$, $i = 1, 2$ such that

$$c_k^h \quad \text{converges weakly-star to} \quad c \quad \text{in} \quad L^\infty(0,T,H^1(\Omega)), \tag{1.35}$$
$$\widehat{c}_k^h \quad \text{converges weakly-star to} \quad \widehat{c} \quad \text{in} \quad L^\infty(0,T,H^1(\Omega)), \tag{1.36}$$
$$\sqrt{t}\partial_t\widehat{c}_k^h \quad \text{converges weakly to} \quad \sqrt{t}\partial_t\widehat{c} \quad \text{in} \quad L^2(0,T,H^1(\Omega)), \tag{1.37}$$
$$\theta_{ik}^h \quad \text{converges weakly-star to} \quad \theta_i \quad \text{in} \quad L^\infty(0,T,H^1(\Omega)), \tag{1.38}$$
$$\widehat{\theta}_{ik}^h \quad \text{converges weakly-star to} \quad \widehat{\theta}_i \quad \text{in} \quad L^\infty(0,T,H^1(\Omega)), \tag{1.39}$$
$$\sqrt{t}\partial_t\widehat{\theta}_{ik}^h \quad \text{converges weakly to} \quad \sqrt{t}\partial_t\widehat{\theta}_i \quad \text{in} \quad L^2(0,T,H^1(\Omega)), \tag{1.40}$$
$$\sqrt{t}w_k^h \quad \text{converges weakly-star to} \quad \sqrt{t}w \quad \text{in} \quad L^\infty(0,T,H^1(\Omega)), \tag{1.41}$$
$$\mathcal{F}_{hk}^c \quad \text{converges weakly-star to} \quad \mathcal{F}^c \quad \text{in} \quad L^\infty(0,T,L^2(\Omega)), \tag{1.42}$$
$$\mathcal{F}_{hk}^{\theta_i} \quad \text{converges weakly-star to} \quad \mathcal{F}^{\theta_i} \quad \text{in} \quad L^\infty(0,T,L^2(\Omega)).$$

Moreover, by calling $\Omega_T = \Omega \times (0,T)$ and observing that

$$||\widehat{c}_k^h - c_k^h||^2_{L^2(\Omega_T)} = \sum_{r=1}^N \int_{(r-1)k}^{rk} |\widehat{c}_k^h - c_k^h|^2 dt \le k\left[k^2 \sum_{r=1}^N |\partial C^r|^2\right],$$

it results from (1.30) that $\widehat{c} = c$. In the same way, (1.31) and

$$||\widehat{\theta}_{ik}^h - \theta_{ik}^h||^2_{L^2(\Omega_T)} \le k \sum_{r=1}^N |\Theta_i^r - \Theta_i^{r-1}|^2 = k^2\left[k \sum_{r=1}^N |\partial\Theta_i^r|^2\right]$$

imply that $\widehat{\theta}_1 = \theta_1$ and $\widehat{\theta}_2 = \theta_2$.

We also observe that for $\xi \in C^\infty(0,T)$, as k goes to zero, we have that

$$\xi_k \quad \text{converges to} \quad \xi \quad \text{in} \quad L^2(0,T),$$
$$\widehat{\xi}_k' \quad \text{converges to} \quad \xi' \quad \text{in} \quad L^2(0,T).$$

To prove that we obtain a solution in the limit, we proceed as follows. Given $\eta \in H^1(\Omega)$, we set $\chi = R^h \eta$ and multiply equations (1.14) and (1.15) by $k\xi^{n-1}$ to get

$$-k[\partial \xi^n](C^n, \chi) + \xi^n(C^n, \chi) - \xi^{n-1}(C^{n-1}, \chi) + k\xi^{n-1}(\nabla W^n, \nabla \chi) = 0,$$
$$k\xi^{n-1}(W^n, \chi) - kD\xi^{n-1}\Big(\partial_c \mathcal{F}(C^n, \Theta_1^n, \Theta_2^n), \chi\Big) - k\lambda_c D\xi^{n-1}(\nabla C^n, \nabla \chi) = 0.$$

By summing over n the previously resulting equations, we obtain

$$-k\sum_{r=1}^{N-1}[\partial \xi^r](C^r, \chi) - \xi^N(C^N, \chi) + \xi^{N-1}(C^N, \chi) + \xi^N(C^N, \chi) - \xi^0(C^0, \chi)$$
$$+k\sum_{r=1}^{N} \xi^{r-1}(\nabla W^r, \nabla \chi) = 0,$$
$$k\sum_{r=1}^{N} \xi^{r-1}\Big[\Big(W^r - D\partial_c \mathcal{F}(C^r, \Theta_1^r, \Theta_2^r), \chi\Big) - \lambda_c D(\nabla C^r, \nabla \chi)\Big] = 0$$

or, equivalently,

$$-\int_0^T [\widehat{\xi}_k'(t)(c_k^h, \chi) + \xi_k(t)(\nabla w_k^h, \nabla \chi)]dt + \xi^{N-1}(C^N, \chi) - \xi^0(c_0, \chi) = 0$$

and

$$\int_0^T \xi_k\Big[\Big(w_k^h - D\mathcal{F}_{hk}^c, \chi\Big) - \lambda_c D(\nabla c_k^h, \nabla \chi)\Big]dt = 0.$$

Choosing ξ such that $\xi(T) = 0$ and $\xi(0) \neq 0$, using the bounds on $\sqrt{t}w_k^h$, c_k^h and $\mathcal{F}_{hk}^c$ and observing that $||\chi||_{H^1(\Omega)}$ remains bounded as k, h go to zero and ξ^{N-1} converges to $\xi(T)$, we can pass to the limit to obtain

$$-\int_0^T [\xi'(t)(c, \eta) + \xi(t)(\nabla w, \nabla \eta)]dt - \xi(0)(c_0, \eta) = 0, \tag{1.43}$$

$$\int_0^T \xi(t)\Big[\Big(w - D\mathcal{F}^c, \eta\Big) - \lambda_c D(\nabla c, \nabla \eta)\Big]dt = 0$$

which implies

$$\langle \partial_t c, \eta \rangle + (\nabla w, \nabla \eta) = 0 \qquad \text{a.e. in} \quad (0, T),$$

$$\Big(w - D\mathcal{F}^c, \eta\Big) - \lambda_c D(\nabla c, \nabla \eta) \qquad \text{a.e. in} \quad (0, T).$$

An integration by parts of (1.43) gives

$$(c(0) - c_0, \eta) = 0 \qquad \forall \eta \in H^1(\Omega)$$

and we conclude that $c(0) = c_0$

It remains to show that

$$\mathcal{F}^c = \partial_c \mathcal{F}(c, \theta_1, \theta_2) \qquad \text{and} \qquad \mathcal{F}^{\theta_i} = \partial_{\theta_i} \mathcal{F}(c, \theta_1, \theta_2), \ i = 1, 2. \tag{1.44}$$

In order to obtain the first equality in (1.44), we argue as Copetti & Elliott (1992). We start defining, for given $M > 0$,

$$F_M(f) = \max\{-M, \min\{M, f\}\} \qquad \text{and} \qquad \phi_M(u, v_1, v_2) = F_M\Big(\partial_c \mathcal{F}(u, v_1, v_2)\Big).$$

To obtain (1.44), we first show that, in some weak sense, the truncation of the sequence $(\mathcal{F}^c_{hk})$ converges to the truncation of $\partial_c \mathcal{F}(c, \theta_1, \theta_2)$ when h and k go to zero. That is, for each M, $F_M(\mathcal{F}^c_{hk})$ converges to $\phi_M(c, \theta_1, \theta_2)$. To conclude the proof, we show that when M goes to infinity, $\phi_M(c, \theta_1, \theta_2)$ converges in a suitable weak sense to $\mathcal{F}^c$. Since it also converges to $\partial_c \mathcal{F}(c, \theta_1, \theta_2)$ this will give the desired identification

For this, let $\tau > 0$, and observe that $\widehat{c}^h_k, \widehat{\theta}^h_{ik}$ are uniformly bounded in $H^1((\tau, T) \times \Omega)$. Since the injection of $H^1((\tau, T) \times \Omega)$ into $L^2((\tau, T) \times \Omega)$ is compact, such estimates guarantee the existence of some subsequences c^h_k and θ^h_{ik} such that

$$c^h_k \text{ converges to } c \quad \text{and} \quad \theta^h_{ik} \text{ converges to } \theta_i \quad \text{in } L^2(\tau, T, L^2(\Omega)) \text{ strongly.} \tag{1.45}$$

Now, let us observe that for $t_{n-1} < t < t_n$ it holds that

$$\begin{aligned}
&\Big[F_M\Big(\mathcal{F}^c_{hk}\Big) - \phi_M(c^h_k, \theta^h_{1k}, \theta^h_{2k})\Big](x) \\
&\qquad = \Big[F_M\Big(\partial_c \mathcal{F}(C^n, \Theta^n_1, \Theta^n_2)\Big) - \phi_M(C^n, \Theta^n_1, \Theta^n_2)\Big](x) \\
&\qquad = \Big[F_M\Big(\partial_c \mathcal{F}(C^n, \Theta^n_1, \Theta^n_2)\Big) - F_M\Big(\partial_c \mathcal{F}(C^n, \Theta^n_1, \Theta^n_2)\Big)\Big](x) = 0.
\end{aligned}$$

We also have

$$\begin{aligned}
&\left|\int_\tau^T \xi(t)\Big(F_M\Big(\mathcal{F}^c_{hk}\Big) - \phi_M(c,\theta_1,\theta_2),\eta\Big)dt\right| \\
&= \left|\int_\tau^T \xi(t)([\phi_M(c^h_k,\theta^h_{1k},\theta^h_{2k}) - \phi_M(c,\theta_1,\theta_2)] + [F_M(\mathcal{F}^c_{hk}) - \phi_M(c^h_k,\theta^h_{1k},\theta^h_{2k})],\eta)dt\right| \\
&= \left|\int_\tau^T \xi(t)(\phi_M(c^h_k,\theta^h_{1k},\theta^h_{2k}) - \phi_M(c,\theta_1,\theta_2),\eta)dt\right|. \qquad (1.46)
\end{aligned}$$

By using the fact that ϕ_M is Lipschitz continuous, it results that

$$\left|\int_\tau^T \xi(t)(\phi_M(c^h_k,\theta^h_{1k},\theta^h_{2k}) - \phi_M(c,\theta_1,\theta_2),\eta)dt\right| \leq C\int_\tau^T |\xi(t)|\left[|c^h_k - c| + \sum_{i=1}^2 |\theta^h_{ik} - \theta_i|\right]|\eta|dt.$$

Since (1.45) holds true, the right hand side of the above expression tends to zero as k, h go to zero. Therefore, taking the limit in (1.46) when k, h go to zero, we obtain

$$\left|\int_\tau^T \xi(t)\Big(F_M\Big(\mathcal{F}^c_{hk}\Big),\eta\Big)dt\right| \quad \text{converges to} \quad \left|\int_\tau^T \xi(t)\Big(\phi_M(c,\theta_1,\theta_2),\eta\Big)dt\right|. \qquad (1.47)$$

Now, we derive some estimates to pass to the limit in M. Defining $\Omega^{h,k}_M = \Big\{x,\ \Big|\mathcal{F}^c_{hk}(x,t)\Big| > M\Big\}$, it follows from the boundedness of $\mathcal{F}^c_{hk}$ in $L^\infty(0,T,L^2(\Omega))$ that

$$\int_{\Omega^{h,k}_M}\Big|\mathcal{F}^c_{hk}(x,t)\Big|^2 dx \leq |\mathcal{F}^c_{hk}(t)|^2 \leq C,$$

which yields

$$|\Omega^{h,k}_M| \leq \frac{C}{M^2}.$$

Thus, for all $\eta \in L^\infty(\Omega)\cap H^1(\Omega)$ and $\tau > 0$, we have

$$\begin{aligned}
\left|\int_\tau^T \xi(t)\Big(\mathcal{F}^c_{hk} - F_M\Big(\mathcal{F}^c_{hk}\Big),\eta\Big)dt\right| &= \left|\int_\tau^T \xi(t)\int_{\Omega^{h,k}_M}\Big[\mathcal{F}^c_{hk} - F_M\Big(\mathcal{F}^c_{hk}\Big)\Big]\eta dxdt\right| \\
&\leq \|\xi\|_\infty\|\eta\|_\infty \int_\tau^T\int_{\Omega^{h,k}_M}\Big[\Big|\mathcal{F}^c_{hk}\Big| + M\Big]dxdt \\
&\leq \|\xi\|_\infty\|\eta\|_\infty\left(\int_\tau^T |\Omega^{h,k}_M|^{1/2}|\mathcal{F}^c_{hk}|dt + \frac{CT}{M}\right)
\end{aligned}$$

and the boundedness of $\mathcal{F}^c_{hk}$ in $L^\infty(0,T,L^2(\Omega))$ yields

$$\left|\int_\tau^T \xi(t)\Big(\mathcal{F}^c_{hk} - F_M\Big(\mathcal{F}^c_{hk}\Big),\eta\Big)\,dt\right| \le \frac{C}{M}\|\xi\|_\infty\|\eta\|_\infty.$$

Thus, with the convergences given by (1.42) and (1.47) when k,h go to zero, we obtain

$$\left|\int_\tau^T \xi(t)\Big(\mathcal{F}^c - \phi_M(c,\theta_1,\theta_2),\eta\Big)\,dt\right| \le \frac{C}{M}\|\xi\|_\infty\|\eta\|_\infty \tag{1.48}$$

Since the regularities of c,θ_1 and θ_2 imply that $\partial_c\mathcal{F}(c,\theta_1,\theta_2)\in L^2(\Omega_T)$, as M goes to infinity, we have that

$$\phi_M(c,\theta_1,\theta_2) \quad \text{converges to} \qquad \partial_c\mathcal{F}(c,\theta_1,\theta_2) \quad \text{in} \quad L^2(\tau,T,L^2(\Omega));$$

and (1.48) gives

$$\mathcal{F}^c = \partial_c\mathcal{F}(c,\theta_1,\theta_2) \text{ in } (\tau,T).$$

Since τ is arbitrary, (1.44) follows.

Using similar arguments, we can pass to the limit in the equations for the crystallographic variables θ_i. For this, given $\eta\in H^1(\Omega)$, we set $\mu = R^h\eta$ and from equation (1.17), we can pass to the limit as k,h go to zero to obtain

$$-\int_0^T \{\xi'(t)(\theta_i,\mu) + \xi(t)[\lambda_i L_i(\nabla\theta_i,\nabla\mu) + L_i(\mathcal{F}^{\theta_i},\mu)]\}dt - \xi^0(\theta_{i0},\mu) = 0, \tag{1.49}$$

which implies

$$\langle\partial_t\theta_i,\eta\rangle + L_i\lambda_i(\nabla\theta_i,\nabla\eta) + L_i\Big(\mathcal{F}^{\theta_i},\eta\Big) = 0 \quad \text{a.e. in } \ (0,T).$$

An integration by parts in (1.49) gives

$$(\theta_i(0)-\theta_{i0},\eta) = 0 \qquad \forall\eta\in H^1(\Omega),$$

and, therefore, $\theta_i(0)=\theta_{i0},\ i=1,2$.

To obtain the remaining identifications in (1.44), we proceed as before. For given $M>0$, we define

$$F_M(f) = \max\{-M,\min\{M,f\}\}, \qquad \psi_M(u,v_1,v_2) = F_M\Big(\partial_{\theta_i}\mathcal{F}(u,v_1,v_2)\Big)$$

and

$$\Omega_M^{h,k} = \Big\{x, \ \Big|\mathcal{F}\theta_k^h(x,t)\Big| > M\Big\}.$$

Similarly as before, we can show that

$$\mathcal{F}^{\theta_1} = \partial_{\theta_1}\mathcal{F}(c,\theta_1,\theta_2) \qquad \text{and} \qquad \mathcal{F}^{\theta_2} = \partial_{\theta_2}\mathcal{F}(c,\theta_1,\theta_2).$$

We conclude that the previous limit functions correspond in fact to a solution of (1.11)–(1.13) in the case when $p = 2$. The case when $p > 2$ is similar.

Since by Proposition 1.1 below there is at most one such solution, by standard argument, we conclude that the whole sequence of approximate solutions converges. Thus we have the following result:

THEOREM 1.3 The sequence of approximate solutions constructed in Section 1.3 converges to the solution of (1.11)–(1.13) in the sense presented in (1.35)–(1.41).

1.5 Uniqueness

In this section, we conclude the proof of Theorem 1.1 establishing the uniqueness.

PROPOSITION 1.1 Under the hypotheses stated in Theorem 1.1, (1.11)–(1.13) has at most one solution.

Proof. We will use an idea similar to that in Elliott & Luckhaus (1991). Let $u \in [H^1(\Omega)]'$, be such that $\langle u, 1\rangle = 0$. We introduce the Green's operator $\mathcal{G}$ defined by:

$$\mathcal{G}u \in H^1(\Omega), \qquad \int_\Omega \mathcal{G}u = 0,$$
$$(\nabla\mathcal{G}u, \nabla\eta) = \langle u, \eta\rangle, \quad \forall \eta \in H^1(\Omega),$$

where $\langle\cdot,\cdot\rangle$ denotes the duality pairing between $H^1(\Omega)$ and its dual.

Let $z^c = c^1 - c^2, z^w = w^1 - w^2$ and $z^{\theta_i} = \theta_i^1 - \theta_i^2$, $i = 1,\dots,p$ be the differences of two pair of solutions to (1.11)–(1.13) as in Theorem 1.1. By taking such differences as multipliers, we find from (1.12)–(1.13) that

$$D\lambda_c|\nabla z^c|^2 = \Big(z^w, z^c\Big) - D\Big(\partial_c\mathcal{F}(c^1,\theta_1^1,\dots,\theta_p^1) - \partial_c\mathcal{F}(c^2,\theta_1^2,\dots,\theta_p^2), z^c\Big),$$

$$\frac{D}{2L_i}\frac{d}{dt}|z^{\theta_i}|^2 + D\lambda_i|\nabla z^{\theta_i}|^2 + D\Big(\partial_{\theta_i}\mathcal{F}(c^1,\theta_1^1,\dots,\theta_p^1) - \partial_{\theta_i}\mathcal{F}(c^2,\theta_1^2,\dots,\theta_p^2), z^{\theta_i}\Big) = 0,$$

for $i = 1, \dots, p$. By adding the above equations, using (1.9), (1.10) and the convexity of the function $[\mathcal{F} + H](c, \theta_1, \dots, \theta_p)$ with

$$H(c, \theta_1, \dots, \theta_p) = \frac{A}{2}(c - c_m)^2 + \gamma \sum_{i=1}^{p} g(c, \theta_i) - \sum_{i=1}^{p} \sum_{i \neq j=1}^{p} \varepsilon_{ij} f(\theta_i, \theta_j),$$

we obtain

$$D\lambda_c |\nabla z^c|^2 + \sum_{i=1}^{p} \frac{D}{2L_i} \frac{d}{dt} |z^{\theta_i}|^2 + D \sum_{i=1}^{p} \lambda_i |\nabla z^{\theta_i}|^2$$

$$\leq \left(z^w, z^c\right) + [A + 2p\gamma G_1]|z^c|^2 + \sum_{i=1}^{p} 2[\gamma G_2 + \overline{\varepsilon}(p-1)(F_1 + F_2)]|z^{\theta_i}|^2,$$

where $\overline{\varepsilon} = \max\{\varepsilon_{ij}\}$ and F_1, F_2, G_1 and G_2 are as in (1.9) and (1.10). We observe that since the average of c is conserved, we have $(z^c, 1) = 0$. By (1.11), we have

$$\overline{z^w} = -\mathcal{G} z_t^c \qquad \text{and} \qquad |z^c|^2 = (\nabla \mathcal{G} z^c, \nabla z^c).$$

Therefore, $\left(z^w, z^c\right) = \left(\overline{z^w}, z^c\right) = -(\nabla \mathcal{G} z_t^c, \nabla \mathcal{G} z^c)$ and we have

$$\frac{1}{2} \frac{d}{dt} |\nabla \mathcal{G} z^c|^2 + \sum_{i=1}^{p} \frac{D}{2L_i} \frac{d}{dt} |z^{\theta_i}|^2 \leq \frac{A + 2p\gamma G_1}{4D\lambda_c} |\nabla \mathcal{G} z^c|^2 + \sum_{i=1}^{p} 2[\gamma G_2 + \overline{\varepsilon}(p-1)(F_1 + F_2)]|z^{\theta_i}|^2.$$

A standard Gronwall argument then yields $\nabla \mathcal{G} z^c = 0$ and $z^{\theta_i} = 0$ since

$$z^c(0) = 0 \qquad \text{and} \qquad z^{\theta_i}(0) = 0, \quad i = 1, \dots, p.$$

Since $|z^c|^2 = (\nabla \mathcal{G} z^c, \nabla z^c) = 0$, we have $z^c = 0$.

Finally, the uniqueness follows from the fact that (1.12) together $z^c = 0$ and $z^{\theta_i} = 0$ imply that $|z^w|^2 = 0$. ■

Theorem 1.1 is now consequence of the previous results.

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Bibliografia

Chen, L.-Q. & Fan, D. 1996 Computer simulation for a coupled grain growth and Ostwald ripening–application to Al_2O_3–Zr_2 two-phase systems. *J. Amer. Ceram. Soc.*, **79**, 1163–1168.

Chen, L.-Q. & Fan, D. 1997*a* Computer simulation of grain growth using a continuum filed model. *Acta Mater.*, **45**, 611–622.

Chen, L.-Q. & Fan, D. 1997*b* Diffusion-controlled grain growth in two-phase solids. *Acta Mater.*, **45**, 3297–3310.

Chen, L.-Q., Fan, D. & Geng, C. 1997 Computer simulation of topological evolution in 2-d grain growth using a continuum diffusion-interface filed model. *Acta Mater.*, **45**, 1115–1126.

Copetti, M. I. M. & Elliott, C. M. 1992 Numerical analysis of the Cahn-Hilliard equation with a logarithmic free energy. *Numer. Math.*, **63**, 39–65.

Elliott, C. M. & Luckhaus, S. 1991 A generalised diffusion equation for phase separation of a multi-component mixture with interfacial free energy. Preprint **887**, IMA (Minnesota).

Fan, D., Chen, L.-Q., Chen, S. & Voorhees, P. W. 1998 Phase field formulations for modelling the Ostwald ripening in two-phase systems. *Comp. Mater. Sci.*, **9**, 329–336.

Capítulo 2

Uma Solução Generalizada de um Modelo para "Ostwald Ripening"

Resumo

Analisamos um sistema não linear formado por uma equação do tipo Cahn-Hilliard e várias do tipo Allen-Cahn. Tal sistema foi proposto por Fan, L.-Q. Chen, S. Chen e Voorhees para modelar o fenômeno de "Ostwald ripening" em sistemas bifásicos. Provamos existência e unicidade de uma solução generalizada do sistema não linear cuja componente de concentração está em L^∞.

A Generalized Solution of a Model for Ostwald Ripening

Patrícia Nunes da Silva
nunes@ime.unicamp.br

José Luiz Boldrini
boldrini@ime.unicamp.br

Abstract

We analyze a system consisting of a Cahn-Hilliard and several Allen-Cahn type equations. This system was proposed by Fan, L.-Q. Chen, S. Chen and Voorhees for modeling Ostwald ripening in two-phase systems. For such system, we prove the existence of a generalized solution whose concentration component is in L^∞.

2.1 Introduction

Ostwald ripening is a phenomenon observed in a wide variety of two-phase systems in which there is coarsening of one phase dispersed in the matrix of another. Because its practical importance, this process has been extensively studied in several degrees of generality. In particular for Ostwald ripening of anisotropic crystals, Fan et al. [6] presented a model taking in consideration both the evolution of the compositional field and of the crystallographic orientations. In the work of Fan et al. [6], there are also numerical experiments used to validate the model, but there is no rigorous mathematical analysis of the model. Our objective in this paper is to do such mathematical analysis.

By defining orientation and composition field variables, the kinetics of coupled grain growth can be described by their spatial and temporal evolution, which is related with the total free energy of the system. The microstructural evolution of Ostwald ripening

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can be described by the Cahn-Hilliard/Allen-Cahn system:

$$\begin{cases} \partial_t c = \nabla \cdot [D\nabla (\partial_c \mathcal{F} - \kappa_c \Delta c)], & (x,t) \in \Omega_T \\ \partial_t \theta_i = -L_i (\partial_{\theta_i} \mathcal{F} - \kappa_i \Delta \theta_i), & (x,t) \in \Omega_T \\ \partial_{\mathbf{n}} c = \partial_{\mathbf{n}} (\partial_c \mathcal{F} - \kappa_c \Delta c) = \partial_{\mathbf{n}} \theta_i = 0, & (x,t) \in S_T \\ c(x,0) = c_0(x), \quad \theta_i(x,0) = \theta_{i0}(x), & x \in \Omega \end{cases} \tag{2.1}$$

for $i = 1, \ldots, p$.

Here, Ω is the physical region where the Ostwald process is occurring; $\Omega_T = \Omega \times (0,T)$; $S_T = \partial\Omega \times (0,T)$; $0 < T < +\infty$; $\mathbf{n}$ denotes the unitary exterior normal vector and $\partial_{\mathbf{n}}$ is the exterior normal derivative at the boundary; $c(x,t)$ is the compositional field (fraction of the soluto with respect to the mixture) which takes the value c_α within the matrix phase, the value c_β ($\neq c_\alpha$) within a second phase grain and intermediate values between c_α and c_β at the interfacial region between the matrix phase and a second phase grain; $\theta_i(x,t)$, for $i = 1, \ldots, p$, are the crystallographic orientations fields; D, κ_c, L_i, κ_i are positive constants related to the material properties. The function $\mathcal{F} = \mathcal{F}(c, \theta_1, \ldots, \theta_p)$ is the local free energy density which is given by

$$\begin{aligned} \mathcal{F}(c, \theta_1, \ldots, \theta_p) = &-\frac{A}{2}(c - c_m)^2 + \frac{B}{4}(c - c_m)^4 + \frac{D_\alpha}{4}(c - c_\alpha)^4 \\ &+\frac{D_\beta}{4}(c - c_\beta)^4 + \sum_{i=1}^{p} \left[-\frac{\gamma}{2}(c - c_\alpha)^2 \theta_i^2 + \frac{\delta}{4}\theta_i^4 \right] + \sum_{i=1}^{p} \sum_{i \neq j=1}^{p} \frac{\varepsilon_{ij}}{2} \theta_i^2 \theta_j^2. \end{aligned} \tag{2.2}$$

where c_α and c_β are the solubilities in the matrix phase and the second phase respectively, and $c_m = (c_\alpha + c_\beta)/2$. The positive coefficients A, B, D_α, D_β, γ, δ and ε_{ij} are phenomenological parameters.

In this paper we obtain a $(p+2)$-tuple which satisfies a variational inequality related to Problem (2.1) and also satisfies the physical requirement that the composition field variable takes values in the closed interval defined by c_α and c_β. That is, the composition field variable should take values in the closure of the set $\{u \in \mathbf{R},\ c_{min} < u < c_{max}\}$ where $c_{min} = \min\{c_\alpha, c_\beta\}$ and $c_{max} = \max\{c_\alpha, c_\beta\}$.

Our approach to the problem is to analyze a three-parameter family of suitable systems which contain a logarithmic perturbation term and approximate the model presented by Fan et al. [6]. In this analysis, we show that the approximate solutions converge to a generalized solution of the original continuous model and this, in particular, will furnish a rigorous proof of the existence of weak solutions (see the statement of Theorem 2.1). Our approach is similar to that used by Passo et al. [3] for an Cahn-Hilliard/Allen-Cahn system with degenerate mobility.

2.2 Existence of Solutions

By making a change of variables in the composition field variable to normalize the interval where the composition field varies, and rescaling the coefficients and the local free energy density, and by using the same notation as before to ease the exposition, we could rewrite (2.1) in the new variable as

$$\begin{cases} \partial_t c = \nabla\left[D\nabla\left(\partial_c \mathcal{F} - \kappa_c \Delta c\right)\right], & (x,t) \in \Omega_T \\ \partial_t \theta_i = -L_i\left(\partial_{\theta_i}\mathcal{F} - \kappa_i \Delta\theta_i\right), & (x,t) \in \Omega_T \\ \partial_{\mathbf{n}} c = \partial_{\mathbf{n}}\left(\partial_c \mathcal{F} - \kappa_c \Delta c\right) = \partial_{\mathbf{n}}\theta_i = 0, & (x,t) \in S_T \\ c(x,0) = c_0(x), \quad \theta_i(x,0) = \theta_{i0}(x), & x \in \Omega \\ 0 \le c \le 1 & (x,t) \in \Omega_T \end{cases} \tag{2.3}$$

for $i = 1, \ldots, p$.

Throughout this paper, standard notation will be used for the required functional spaces. We denote by $\overline{f}$ the mean value of f in Ω of a given $f \in L^1(\Omega)$. We will prove the following:

THEOREM 2.1 Let $T > 0$ and $\Omega \subset R^d$, $1 \le d \le 3$ be a bounded domain with Lipschitz boundary. For all $c_0, \theta_{i0}, i = 1, \ldots, p$, satisfying c_0, $\theta_{i0} \in H^1(\Omega)$, for $i = 1, \ldots, p$, $0 \le c_0 \le 1$ and $\overline{c_0} \in [0,1]$, there exists a unique $(p+2)$-tuple $(c, w - \overline{w}, \theta_1, \ldots, \theta_p)$ such that, for $i = 1, \ldots, p$,
(a) $c,\ \theta_i \in L^\infty(0,T,H^1(\Omega)) \cap L^2(0,T,H^2(\Omega))$,
(b) $w \in L^2(0,T,H^1(\Omega))$;
(c) $\partial_t c \in L^2(0,T,[H^1(\Omega)]')$, $\partial_t \theta_i \in L^2(\Omega_T)$;
(d) $0 \le c \le 1$ a.e. in Ω_T;
(e) $\partial_c \mathcal{F}(c, \theta_1, \ldots, \theta_p)$, $\partial_{\theta_i}\mathcal{F}(c, \theta_1, \ldots, \theta_p) \in L^2(\Omega_T)$;
(f) $c(x,0) = c_0(x)$, $\theta_i(x,0) = \theta_{i0}(x)$;
(g) $\partial_{\mathbf{n}} c_{|S_T} = \partial_{\mathbf{n}} \theta_{i|S_T} = 0$ in $L^2(S_T)$.

(h) We call the $(p+2)$-tuple $(c, w, \theta_1, \dots, \theta_p)$ a generalized solution in the following sense

$$\int_0^T \langle \partial_t c, \phi \rangle dt = -\iint_{\Omega_T} \nabla w \nabla \phi, \quad \forall \phi \in L^2(0,T,H^1(\Omega)), \tag{2.4}$$

$$\int_0^T \xi(t) \left\{ \kappa_c D(\nabla c, \nabla\phi - \nabla c) - (w - D\partial_c \mathcal{F}(c, \theta_1, \dots, \theta_p), \phi - c) \right\} dt \geq 0, \tag{2.5}$$

$\forall \xi \in C[0,T), \xi \geq 0,\ \forall \phi \in K = \{\eta \in H^1(\Omega),\ 0 \leq \eta \leq 1, \overline{\eta} = \overline{c_0}\}$, and

$$\iint_{\Omega_T} \partial_t \theta_i \psi_i = -\iint_{\Omega_T} L_i(\partial_{\theta_i}\mathcal{F}(c, \theta_1, \dots, \theta_p) - \kappa_i \Delta\theta_i)\psi_i, \tag{2.6}$$

$\forall \psi_i \in L^2(\Omega_T), i = 1, \dots, p$, and where $\mathcal{F}$ is given by (2.2), $\langle \cdot, \cdot \rangle$ denotes the duality pairing between $H^1(\Omega)$ and its dual and $(\cdot,\cdot)$ denotes the inner product in $L^2(\Omega)$.

REMARK.

(i). The inequality obtained in (2.5) is similar to one obtained by Elliott and Luckhaus [5] in the case of the deep quench limit problem for a system of nonlinear diffusion equations.

(ii). We observe that (2.5) comes from the fact that classically w is expected to be equal to $D(\partial_c \mathcal{F} - \kappa_c \Delta c)$ up to a constant.

(iii). The solution presented in Theorem 2.1 is a generalized solution of (2.3). In fact, if we had higher regularity for this solution, we could obtain that (2.5) holds as an equality in the region where $0 < c(x,t) < 1$. This can be rigorously obtained in the one-dimensional case (see Remark at the end of the paper).

The above uniqueness is proved below.

LEMMA 2.1 Under the hypotheses stated in Theorem 2.1, in the $(p+2)$-tuple which solves (2.4)–(2.6), the components $c, \theta_1, \dots, \theta_p$ are uniquely determined and the component w is uniquely determined up to a constant.

Proof. We argue as Elliott and Luckhaus [5]. We introduce the Green's operator G: given $f \in [H^1(\Omega)]'_{null} = \{f \in [H^1(\Omega)]',\ \langle f, 1\rangle = 0\}$, we define $Gf \in H^1(\Omega)$ as the unique solution of

$$\int_\Omega \nabla Gf \nabla\psi = \langle f, \psi \rangle, \quad \forall \psi \in H^1(\Omega) \qquad \text{and} \qquad \int_\Omega Gf = 0.$$

Let $z^c = c_1 - c_2$, $z^w = w_1 - w_2$ and $z^{\theta_i} = \theta_{i1} - \theta_{i2}$, $i = 1, \dots, p$ be the differences of two pair of solutions to (2.4)–(2.6) as in Theorem 2.1. Since equation (2.4) implies that the mean value of the composition field in Ω is conserved, we have that $(z^c, 1) = 0$ and we find from (2.4) that

$$-Gz_t^c = \overline{z^w}.$$

The definition of the Green operator and the fact that $(z^c, 1) = 0$ give

$$-(\nabla G z_t^c, \nabla G z^c) = -(G z_t^c, z^c) = (\overline{z^w}, z^c) = (z^w, z^c).$$

We find from (2.5) that

$$-\kappa_c D|\nabla z^c|^2 + (z^w, z^c) - D(\partial_c \mathcal{F}(c_1, \theta_{11}, \dots, \theta_{p1}) - \partial_c \mathcal{F}(c_2, \theta_{12}, \dots, \theta_{p2}), z^c) \geq 0.$$

Thus, we have

$$\frac{1}{2}\frac{d}{dt}|\nabla G z^c| + \kappa_c D|\nabla z^c|^2 \leq -D(\partial_c \mathcal{F}(c_1, \theta_{11}, \dots, \theta_{p1}) - \partial_c \mathcal{F}(c_2, \theta_{12}, \dots, \theta_{p2}), z^c).$$

We find from (2.6) that

$$\frac{D}{2L_i}\frac{d}{dt}|z^{\theta_i}|^2 + D\kappa_i|\nabla z^{\theta_i}|^2 + D\big(\partial_{\theta_i}\mathcal{F}(c_1, \theta_{11}, \dots, \theta_{p1}) - \partial_{\theta_i}\mathcal{F}(c_2, \theta_{12}, \dots, \theta_{p2}), z^{\theta_i}\big) = 0.$$

By adding the above equations, using the convexity of the function $[\mathcal{F} + H](c, \theta_1, \dots, \theta_p)$ with

$$H(c, \theta_1, \dots, \theta_p) = \frac{A}{2}(c - c_m)^2 + \frac{\gamma}{2}\sum_{i=1}^{p}(c - c_\alpha)^2\theta_i^2 - \sum_{i=1}^{p}\sum_{i \neq j = 1}^{p}\frac{\varepsilon_{ij}}{2}\theta_i^2\theta_j^2,$$

and integrating by parts, we obtain

$$\begin{aligned} &\frac{1}{2}\frac{d}{dt}|\nabla \mathcal{G} z^c|^2 + \kappa_c D|\nabla z^c|^2 + \sum_{i=1}^{p}\left[\frac{D}{2L_i}\frac{d}{dt}|z^{\theta_i}|^2 + D\kappa_i|\nabla z^{\theta_i}|^2\right] \\ &\leq \big(\nabla(H(c_1, \theta_{11}, \dots, \theta_{p1}) - H(c_2, \theta_{12}, \dots, \theta_{p2})) \cdot (z^c, z^{\theta_1}, \dots, z^{\theta_p}), 1\big) \end{aligned} \tag{2.7}$$

In order to estimate the term at the right hand side of the above inequality, we use the regularity of c_k and θ_{ik} to obtain

$$\gamma(\nabla(c_1^2\theta_{i1}^2 - c_2^2\theta_{i2}^2) \cdot (z^c, z^{\theta_i}), 1) \leq C[|z^c|^2 + |z^{\theta_i}|^2] + \frac{\kappa_c D}{2p}|\nabla z^c|^2 + \frac{D\kappa_i}{4}|\nabla z^{\theta_i}|^2$$

and

$$\varepsilon_{ij}(\nabla(\theta_{i1}^2\theta_{j1}^2 - \theta_{i2}^2\theta_{j2}^2)\cdot(z^{\theta_i}, z^{\theta_j}), 1) \leq C[|z^{\theta_i}|^2 + |z^{\theta_j}|^2] + \frac{D\kappa_i}{8(p-1)}|\nabla z^{\theta_i}|^2 + \frac{D\kappa_j}{8(p-1)}|\nabla z^{\theta_j}|^2.$$

The above inequalities together (2.7) imply that

$$\frac{1}{2}\frac{d}{dt}|\nabla\mathcal{G}z^c|^2 + \frac{\kappa_c D}{2}|\nabla z^c|^2 + \sum_{i=1}^{p}\left[\frac{D}{2L_i}\frac{d}{dt}|z^{\theta_i}|^2 + \frac{D\kappa_i}{2}|\nabla z^{\theta_i}|^2\right]$$
$$\leq C\left[\|z^c\|_{L^2(\Omega)}^2 + \sum_{i=1}^{p}\|z^{\theta_i}\|_{L^2(\Omega)}^2\right].$$

From the definition of the Green operator, we have that $|z^c|^2 = (\nabla\mathcal{G}z^c, \nabla z^c)$. Using the Hölder inequality, we can rewrite the above inequality as

$$\frac{1}{2}\frac{d}{dt}|\nabla\mathcal{G}z^c|^2 + \frac{\kappa_c D}{4}|\nabla z^c|^2 + \sum_{i=1}^{p}\left[\frac{D}{2L_i}\frac{d}{dt}|z^{\theta_i}|^2 + \frac{D\kappa_i}{2}|\nabla z^{\theta_i}|^2\right]$$
$$\leq C\left[\|\nabla\mathcal{G}z^c\|_{L^2(\Omega)}^2 + \sum_{i=1}^{p}\|z^{\theta_i}\|_{L^2(\Omega)}^2\right].$$

A standard Gronwall argument then yields

$$\nabla\mathcal{G}z^c = 0 \qquad \text{and} \qquad z^{\theta_i} = 0, \quad i = 1, \ldots, p,$$

since

$$\mathcal{G}z^c(0) = 0 \qquad \text{and} \qquad z^{\theta_i}(0) = 0, \quad i = 1, \ldots, p.$$

The uniqueness is proved since $|z^c|^2 = (\nabla\mathcal{G}z^c, \nabla z^c) = 0$. Furthermore, (2.4) together $z^c = 0$ imply that $|\nabla z^w|^2 = 0$. ■

As a corollary of this, we have the following:

LEMMA 2.2 Under the conditions of Theorem 2.1, in the cases where $\overline{c_0}$ is either 0 or 1, we have a solution of (2.4)–(2.6).

Proof. In such cases, since $0 \leq c_0(x) \leq 1$, we have in fact that either $c_0(x) = 0$ or $c_0(x) = 1$. Now, take c identically zero or one, respectively. Then, equation (2.4) is trivially satisfied and will imply that w is a constant. Otherwise, (2.5) is also trivially satisfied and to obtain a solution of the problem (2.4)–(2.6), we just have to solve the heat equation (2.6).

∎

Since by the above lemma, we have uniqueness of c, to prove Theorem 2.1, it just remain to deal with the cases where the mean value of the initial condition c_0 is strictly between to zero and one.

Thus, in the following we assume that

$$\begin{aligned} c_0,\ \theta_{i0} \in H^1(\Omega), \quad i = 1, \dots, p, \\ 0 \le c_0 \le 1, \qquad \overline{c_0} \in (0,1), \end{aligned} \tag{2.8}$$

To obtain the result in Theorem 2.1, we approximate system (2.3) by a three-parameter family of suitable systems which contain a logarithmic perturbation term and then pass to the limit. In Section 2.3, we use the results of Passo et al. [3] to construct such perturbed systems and together with some ideas presented by Copetti and Elliott [2] and by Elliott and Luckhaus [5], we take the limit in these systems in the last three sections.

For sake of simplicity of exposition, without loosing generality, we develop the proof for the case of dimension one and for only one orientation field variable, that is, when Ω is a bounded open interval and p is equal to one, and thus we have just one orientation field that we denote θ. In this case, the local free energy density is reduced to

$$\begin{aligned} \mathcal{F}(c,\theta) = &-\frac{A}{2}(c-c_m)^2 + \frac{B}{4}(c-c_m)^4 + \frac{D_\alpha}{4}(c-c_\alpha)^4 + \frac{D_\beta}{4}(c-c_\beta)^4 \\ &-\frac{\gamma}{2}(c-c_\alpha)^2\theta^2 + \frac{\delta}{4}\theta^4. \end{aligned} \tag{2.9}$$

Even though the crossed terms of (2.2) involving the orientation field variables are absent in above expression, when extending the result for p greater than one, they will not bring any difficulty as we point out at the end of the paper.

2.3 Perturbed Systems

In this section we construct a three-parameter family of perturbed systems. The auxiliary parameter M controls a truncation of the local free energy $\mathcal{F}$ which will permit the application of an existence result of Passo et al. [3]. The parameters σ and ε are related with the logarithmic term whose introduction will enable us to guarantee that the composition field variable c takes values in the closure of the set I.

For each positive constants σ, M and $\varepsilon \in (0,1)$, we define the perturbed local free energy density as follows:

$$\mathcal{F}_{\sigma\varepsilon M}(c,\theta) = f(c) + g_M(\theta) + h_M(c,\theta) + \varepsilon[F_\sigma(c) + F_\sigma(1-c)]. \tag{2.10}$$

where the first three terms give a truncation of the original $\mathcal{F}(c,\theta)$ given in (2.9), and the last term is a logarithmic perturbation. To obtain a truncation of the local free energy density, we introduce bounded functions whose summation coincides with $\mathcal{F}$ for $(c,\theta) \in [0,1] \times [-M,M]$. Let f, g_M and h_M be such that

$$f(c) = -\frac{A}{2}(c-c_m)^2 + \frac{B}{4}(c-c_m)^4 + \frac{D_\alpha}{4}(c-c_\alpha)^4 + \frac{D_\beta}{4}(c-c_\beta)^4, \quad 0 \le c \le 1,$$
$$g_M(\theta) = \frac{\delta}{4}h_2^2(M;\theta) \qquad \text{and} \qquad h_M(c,\theta) = h_1(c)h_2(M;\theta)$$

with

$$h_1(c) = -\frac{\gamma}{2}(c-c_\alpha)^2, \quad 0 \le c \le 1,$$
$$h_2(M;\theta) = \theta^2, \quad -M \le \theta \le M.$$

Outside the intervals $[0,1]$ and $[-M,M]$, we extend the above functions to satisfy

$$\|f\|_{C^2(\mathbf{R})} \le U_0, \qquad \|g_M\|_{C^2(\mathbf{R})} \le V_0(M), \tag{2.11}$$
$$\|h_M\|_{C^2(\mathbf{R}^2)} \le Z_0(M), \qquad \|h_1\|_{C^2(\mathbf{R})} \le W_0 \tag{2.12}$$
$$|h_2(M;\theta)| \le K\theta^2, \qquad |h_2'(M;\theta)| \le K|\theta|, \quad \forall M > 0, \quad \forall \theta \in \mathbf{R}, \tag{2.13}$$

where $U_0, W_0, K > 0$ are constants and, for each M, $V_0(M)$ and $Z_0(M)$ are also constants.

We took the logarithmic term $\varepsilon[F_\sigma(c) - F_\sigma(1-c)]$ as in Passo et al. [3]. Let us denote

$$F(s) = s\ln s.$$

For $\sigma \in (0, 1/e)$, we choose $F_\sigma'(s)$ such that

$$F_\sigma'(s) = \begin{cases} \frac{\sigma}{2\sigma - s} + \ln\sigma, & \text{if } s < \sigma, \\ \ln s + 1, & \text{if } \sigma \le s \le 1-\sigma, \\ f_\sigma(s), & \text{if } 1-\sigma < s < 2, \\ 1, & \text{if } s \ge 2, \end{cases}$$

where $f_\sigma \in C^1([1-\sigma, 2])$ is chosen having the following properties:

$$\begin{gathered} f_\sigma \leq F', \quad f'_\sigma \geq 0, \\ f_\sigma(1-\sigma) = F'(1-\sigma), \quad f_\sigma(2) = 1, \\ f'_\sigma(1-\sigma) = F''(1-\sigma), \quad f'_\sigma(2) = 0. \end{gathered}$$

Defining

$$F_\sigma(s) = -\frac{1}{e} + \int_{\frac{1}{e}}^{s} F'_\sigma(\xi)d\xi,$$

we have

$$F_\sigma \in C^2(\mathbf{R}) \qquad \text{and} \qquad F''_\sigma \geq 0.$$

Clearly, $\mathcal{F}_{\sigma\varepsilon M}$ has a lower bound which is independent of σ and ε. We claim that $\mathcal{F}_{\sigma\varepsilon M}$ can also be inferiorly bounded independently of M. To prove this fact, we just have to estimate $g_M(\theta) + h_M(c,\theta)$. We have

$$\begin{aligned} g_M(\theta) + h_M(c,\theta) &= \frac{\delta}{4}h_2^2(M;\theta) + h_1(c)h_2(M;\theta) \\ &= \frac{\delta}{4}h_2(M;\theta)\left[h_2(M;\theta) + \frac{4}{\delta}h_1(c)\right] \geq -\frac{h_1^2(c)}{\delta} \geq -\frac{Z_0^2}{\delta} \end{aligned}$$

Therefore, we have

$$\begin{gathered} -U_0 - \frac{Z_0^2}{\delta} - \frac{2}{e} \leq \mathcal{F}_{\sigma\varepsilon M}(c,\theta) \quad \text{in } \mathbf{R}^2, \\ \mathcal{F}_{\sigma\varepsilon M}(c,\theta) < U_0 + g_M(\theta) - h_M(c,\theta) \quad \text{in } \operatorname{cl} I. \end{gathered} \tag{2.14}$$

The perturbed systems are given by

$$\begin{cases} \partial_t c = D\left(\partial_c \mathcal{F}_{\sigma\varepsilon M}(c,\theta) - \kappa_c c_{xx}\right)_{xx}, & (x,t) \in \Omega_T \\ \partial_t \theta = -L\left[\partial_\theta \mathcal{F}_{\sigma\varepsilon M}(c,\theta) - \kappa\theta_{xx}\right], & (x,t) \in \Omega_T \\ \partial_{\mathbf{n}} c = \partial_{\mathbf{n}}(\partial_c \mathcal{F}_{\sigma\varepsilon M}(c,\theta) - \kappa_c c_{xx}) = \partial_{\mathbf{n}}\theta = 0, & (x,t) \in S_T \\ c(x,0) = c_0(x), \quad \theta(x,0) = \theta_0(x), & x \in \Omega \end{cases} \tag{2.15}$$

To solve the above problem, we shall use the next proposition which is an existence result stated by Passo et al. [3] to the following system:

$$\begin{cases} \partial_t u = \left[q_1(u,v)\left(f_1(u,v) - \kappa_1 u_{xx}\right)_x\right]_x, & (x,t) \in \Omega_T \\ \partial_t v = -q_2(u,v)\left[f_2(u,v) - \kappa_2 v_{xx}\right], & (x,t) \in \Omega_T \\ \partial_{\mathbf{n}} u = \partial_{\mathbf{n}} u_{xx} = \partial_{\mathbf{n}} v = 0, & (x,t) \in S_T \\ u(x,0) = u_0(x), \quad v(x,0) = v_0(x), & x \in \Omega \end{cases} \tag{2.16}$$

where q_i and f_i satisfy:

(H1) $q_i \in C(\mathbf{R}^2, \mathbf{R}^+)$, with $q_{\min} \leq q_i \leq q_{\max}$ for some $0 < q_{\min} \leq q_{\max}$;
(H2) $f_1 \in C^1(\mathbf{R}^2, \mathbf{R})$ and $f_2 \in C(\mathbf{R}^2, \mathbf{R})$, with $\|f_1\|_{C^1} + \|f_2\|_{C^0} \leq F_0$ for some $F_0 > 0$.

Proposition 2.1 Assuming (H1), (H2) and $u_0,\ v_0 \in H^1(\Omega)$, there exists a pair of functions (u,v) such that:

(i). $u \in L^\infty(0,T,H^1(\Omega)) \cap L^2(0,T,H^3(\Omega)) \cap C([0,T];H^\lambda(\Omega))$, $\lambda < 1$

(ii). $v \in L^\infty(0,T,H^1(\Omega)) \cap L^2(0,T,H^2(\Omega)) \cap C([0,T];H^\lambda(\Omega))$, $\lambda < 1$

(iii). $\partial_t u \in L^2(0,T,[H^1(\Omega)]')$, $\quad \partial_t v \in L^2(\Omega_T)$

(iv). $u(0) = u_0$ and $v(0) = v_0$ in $L^2(\Omega)$

(v). $\partial_{\mathbf{n}} u_{|S_T} = \partial_{\mathbf{n}} v_{|S_T} = 0$ in $L^2(S_T)$

(vi). (u,v) solves (2.16) in the following sense:

$$\int_0^t \langle \partial_t u, \phi\rangle = -\iint_{\Omega_t} q_1(u,v)(f_1(u,v) - \kappa_1 u_{xx})_x \phi_x, \quad \forall \phi \in L^2(0,T,H^1(\Omega))$$

$$\iint_{\Omega_t} \partial_t v \psi = -\iint_{\Omega_t} q_2(u,v)(f_2(u,v) - \kappa_2 v_{xx})\psi, \quad \forall \psi \in L^2(\Omega_T).$$

Remark. The regularity of the test functions with respect to t allow us to obtain the integrals over $(0,t)$, instead of $(0,T)$ as originally presented by Passo et al. [3].

Applying the above proposition, for each $\varepsilon, \sigma, M > 0$ there exists a solution $(c_{\sigma\varepsilon M}, \theta_{\sigma\varepsilon M})$ of Problem (2.15) in the following sense

$$\int_0^t \langle \partial_t c_{\sigma\varepsilon M}, \phi\rangle = -\iint_{\Omega_t} D(\partial_c \mathcal{F}_{\sigma\varepsilon M}(c_{\sigma\varepsilon M}, \theta_{\sigma\varepsilon M}) - \kappa_c [c_{\sigma\varepsilon M}]_{xx})_x \phi_x, \tag{2.17}$$

for $\phi \in L^2(0,T,H^1(\Omega))$ and

$$\iint_{\Omega_t} \partial_t \theta_{\sigma\varepsilon M} \psi = -\iint_{\Omega_t} L(\partial_\theta \mathcal{F}_{\sigma\varepsilon M}(c_{\sigma\varepsilon M}, \theta_{\sigma\varepsilon M}) - \kappa[\theta_{\sigma\varepsilon M}]_{xx})\psi, \tag{2.18}$$

for $\psi \in L^2(\Omega_T)$.

Let us observe that equation for c in equation (2.17) implies that the mean value of $c_{\sigma\varepsilon M}$ in Ω is given by

$$\overline{c_{\sigma\varepsilon M}(t)} = \overline{c_0} \in (0,1) \tag{2.19}$$

2.4 Limit as $M \to \infty$

In this section we obtain some a priori estimates that allow taking the limit in the parameter M. Actually, some of these estimates are also independent of the parameters σ and ε and will be useful in next sections.

LEMMA 2.3 There exists a constant C_1 independent of M (sufficiently large), σ (sufficiently small) and ε such that

(i). $\|c_{\sigma\varepsilon M}\|_{L^\infty(0,T,H^1(\Omega))} \leq C_1$

(ii). $\|\theta_{\sigma\varepsilon M}\|_{L^\infty(0,T,H^1(\Omega))} \leq C_1$

(iii). $\|(\partial_c \mathcal{F}_{\sigma\varepsilon M} - \kappa_c(c_{\sigma\varepsilon M})_{xx})_x\|_{L^2(\Omega_T)} \leq C_1$

(iv). $\|\partial_\theta \mathcal{F}_{\sigma\varepsilon M} - \kappa(\theta_{\sigma\varepsilon M})_{xx}\|_{L^2(\Omega_T)} \leq C_1$

(v). $\|\partial_t c_{\sigma\varepsilon M}\|_{L^2(0,T,[H^1(\Omega)]')} \leq C_1$

(vi). $\|\partial_t \theta_{\sigma\varepsilon M}\|_{L^2(\Omega_T)} \leq C_1$

(vii). $\|\mathcal{F}_{\sigma\varepsilon M}(c_{\sigma\varepsilon M}, \theta_{\sigma\varepsilon M})\|_{L^\infty(0,T,L^1(\Omega))} \leq C_1$

Proof. To obtain items (iii), (iv) and (vii), we argue as Passo et al. [3] and Elliott and Garcke [4]. First, we observe that by the regularity of $c_{\sigma\varepsilon M}$ and $\theta_{\sigma\varepsilon M}$, we could take

$$\partial_c \mathcal{F}_{\sigma\varepsilon M} - \kappa_c(c_{\sigma\varepsilon M})_{xx} \quad \text{and} \quad \partial_\theta \mathcal{F}_{\sigma\varepsilon M} - \kappa(\theta_{\sigma\varepsilon M})_{xx}$$

as test functions in the equations (2.17) and (2.18), respectively, to obtain

$$\begin{aligned}&\int_0^t \langle \partial_t c_{\sigma\varepsilon M}, \partial_c \mathcal{F}_{\sigma\varepsilon M} - \kappa_c (c_{\sigma\varepsilon M})_{xx}\rangle + \iint_{\Omega_t} \partial_t \theta_{\sigma\varepsilon M} \partial_\theta \mathcal{F}_{\sigma\varepsilon M} - \kappa(\theta_{\sigma\varepsilon M})_{xx} \\ &= -\iint_{\Omega_t} D[(\partial_c \mathcal{F}_{\sigma\varepsilon M} - \kappa_c (c_{\sigma\varepsilon M})_{xx})_x]^2 - \iint_{\Omega_t} L[\partial_\theta \mathcal{F}_{\sigma\varepsilon M} - \kappa(\theta_{\sigma\varepsilon M})_{xx}]^2.\end{aligned} \tag{2.20}$$

Also, given a small $h > 0$, we consider the functions

$$\mathcal{F}_{\sigma\varepsilon Mh} = \mathcal{F}_{\sigma\varepsilon M}(c_{\sigma\varepsilon Mh}, \theta_{\sigma\varepsilon M}) \qquad \text{and} \qquad c_{\sigma\varepsilon Mh}(t,x) = \frac{1}{h}\int_{t-h}^t c_{\sigma\varepsilon M}(\tau, x) d\tau$$

where we set $c_{\sigma\varepsilon M}(t,x) = c_0(x)$ for $t \leq 0$. Since $\partial_t c_{\sigma\varepsilon Mh}(t,x) \in L^2(\Omega_T)$, we have

$$\begin{aligned}&\int_0^t \langle (c_{\sigma\varepsilon Mh})_t, [\partial_c \mathcal{F}_{\sigma\varepsilon Mh} - \kappa_c (c_{\sigma\varepsilon Mh})_{xx}]\rangle dt + \iint_{\Omega_t} (\theta_{\sigma\varepsilon M})_t [\partial_\theta \mathcal{F}_{\sigma\varepsilon Mh} - \kappa(\theta_{\sigma\varepsilon M})_{xx}] \\ &= \int_\Omega \left[\frac{\kappa_c}{2}|[c_{\sigma\varepsilon Mh}(t)]_x|^2 + \frac{\kappa}{2}|[\theta_{\sigma\varepsilon M}]_x(t)|^2 + \mathcal{F}_{\sigma\varepsilon Mh}(t)\right] \\ &\qquad - \int_\Omega \left[\frac{\kappa_c}{2}|[c_0]_x|^2 + \frac{\kappa}{2}|[\theta_0]_x|^2 + \mathcal{F}_{\sigma\varepsilon M}(c_0, \theta_0)\right].\end{aligned}$$

Taking the limit as h tends to zero in the above expression and using (2.20), we obtain

$$\begin{aligned}&\iint_{\Omega_t} D[(\partial_c \mathcal{F}_{\sigma\varepsilon M} - \kappa_c (c_{\sigma\varepsilon M})_{xx})_x]^2 + \iint_{\Omega_t} L[\partial_\theta \mathcal{F}_{\sigma\varepsilon M} - \kappa(\theta_{\sigma\varepsilon M})_{xx}]^2 \\ &\qquad + \frac{\kappa_c}{2}\|[c_{\sigma\varepsilon M}]_x(t)\|^2_{L^2(\Omega)} + \frac{\kappa}{2}\|[\theta_{\sigma\varepsilon M}]_x(t)\|^2_{L^2(\Omega)} + \int_\Omega \mathcal{F}_{\sigma\varepsilon M}(t) \\ &= \frac{\kappa_c}{2}\|[c_0]_x\|^2_{L^2(\Omega)} + \frac{\kappa}{2}\|[\theta_0]_x\|^2_{L^2(\Omega)} + \int_\Omega \mathcal{F}_{\sigma\varepsilon M}(c_0, \theta_0)\end{aligned}$$

for almost every $t \in (0, T]$. Using (2.8) and (2.14), we could choose M_0 and σ_0, depending only on the initial conditions, to obtain for all $M > M_0$ and all $\sigma < \sigma_0$

$$\begin{aligned}&\iint_{\Omega_T} D[(\partial_c \mathcal{F}_{\sigma\varepsilon M} - \kappa_c (c_{\sigma\varepsilon M})_{xx})_x]^2 + \iint_{\Omega_T} L[\partial_\theta \mathcal{F}_{\sigma\varepsilon M} - \kappa(\theta_{\sigma\varepsilon M})_{xx}]^2 \\ &\qquad + \frac{\kappa_c}{2}\|[c_{\sigma\varepsilon M}]_x(t)\|^2_{L^2(\Omega)} + \frac{\kappa}{2}\|[\theta_{\sigma\varepsilon M}]_x(t)\|^2_{L^2(\Omega)} + \int_\Omega \mathcal{F}_{\sigma\varepsilon M}(t) \leq C_1\end{aligned} \tag{2.21}$$

which implies items (iii), (iv) and (vii) since we have (2.14). Using the Poincaré inequality and (2.19), item (i) is also verified.

To prove item (vi), we choose $\psi = \partial_t\theta_{\sigma\varepsilon M}$ as a test function in (2.18), which yields

$$\iint_{\Omega_T} [\partial_t\theta_{\sigma\varepsilon M}]^2 = -\iint_{\Omega_T} L(\partial_\theta\mathcal{F}_{\sigma\varepsilon M} - \kappa(\theta_{\sigma\varepsilon M})_{xx})\partial_t\theta_{\sigma\varepsilon M}$$
$$\leq \left(\iint_{\Omega_T} L^2(\partial_\theta\mathcal{F}_{\sigma\varepsilon M} - \kappa(\theta_{\sigma\varepsilon M})_{xx})^2\right)^{1/2}\left(\iint_{\Omega_T}[\partial_t\theta_{\sigma\varepsilon M}]^2\right)^{1/2}.$$

Since we have

$$\int_\Omega \theta^2_{\sigma\varepsilon M} \leq 2\int_\Omega |\theta_0|^2 + 2t\iint_{\Omega_T}(\partial_t\theta_{\sigma\varepsilon M})^2 d\tau \leq C_2,$$

item (vi) and (2.21), then item (ii) is verified. Finally, item (v) follows since

$$\left|\int_0^T \langle\partial_t c_{\sigma\varepsilon M}, \phi\rangle\right| \leq \left(\iint_{\Omega_T} D^2[(\partial_c\mathcal{F}_{\sigma\varepsilon M} - \kappa_c(c_{\sigma\varepsilon M})_{xx})_x]^2\right)^{1/2}\left(\iint_{\Omega_T}(\phi_x)^2\right)^{1/2}$$

for all $\phi \in L^2(0,T,H^1(\Omega))$.

Remark. From (2.21), using (2.14), we obtain

$$\begin{aligned}\iint_{\Omega_T} D[(\partial_c\mathcal{F}_{\sigma\varepsilon M} - \kappa_c(c_{\sigma\varepsilon M})_{xx})_x]^2 + \iint_{\Omega_T} L[\partial_\theta\mathcal{F}_{\sigma\varepsilon M} - \kappa(\theta_{\sigma\varepsilon M})_{xx}]^2 \\ + \frac{\kappa_c}{2}\|[c_{\sigma\varepsilon M}(t)]_x\|^2_{L^2(\Omega)} + \frac{\kappa}{2}\|[\theta_{\sigma\varepsilon M}]_x(t)\|^2_{L^2(\Omega)} \leq C_1.\end{aligned} \tag{2.22}$$

Lemma 2.4 For M sufficiently large and σ sufficiently small, there exist a constant C_3 independent of σ, M and ε and a constant $C_3'(\sigma)$ independent of M and ε such that

(i). $\|\partial_c\mathcal{F}_{\sigma\varepsilon M}\|_{L^2(0,T,H^1(\Omega))} \leq C_3'$,

(ii). $\|\partial_\theta\mathcal{F}_{\sigma\varepsilon M}\|_{L^2(\Omega_T)} \leq C_3$,

(iii). $\|[c_{\sigma\varepsilon M}]_{xx}\|_{L^2(\Omega_T)} \leq C_3$,

(iv). $\|[\theta_{\sigma\varepsilon M}]_{xx}\|_{L^2(\Omega_T)} \leq C_3$,

Proof. First, we prove items (ii) and (iv). From Lemma 2.3(iv), we have

$$\iint_{\Omega_T}(\partial_\theta\mathcal{F}_{\sigma\varepsilon M})^2 - 2\kappa\iint_{\Omega_T}\partial_\theta\mathcal{F}_{\sigma\varepsilon M}[\theta_{\sigma\varepsilon M}]_{xx} + \kappa^2\iint_{\Omega_T}[\theta_{\sigma\varepsilon M}]^2_{xx} \leq C_3. \tag{2.23}$$

Since

$$\partial_\theta \mathcal{F}_{\sigma\varepsilon M}[\theta_{\sigma\varepsilon M}]_{xx} = [g'_M(\theta_{\sigma\varepsilon M}) + \partial_\theta h_M(c_{\sigma\varepsilon M}, \theta_{\sigma\varepsilon M})][\theta_{\sigma\varepsilon M}]_{xx}$$
$$= [g'_M(\theta_{\sigma\varepsilon M}) + h_1(c_{\sigma\varepsilon M})h'_2(M;\theta_{\sigma\varepsilon M})][\theta_{\sigma\varepsilon M}]_{xx},$$

using (2.12) and (2.13), we obtain

$$2\kappa\partial_\theta \mathcal{F}_{\sigma\varepsilon M}[\theta_{\sigma\varepsilon M}]_{xx} \leq \frac{\kappa^2}{2}[\theta_{\sigma\varepsilon M}]^2_{xx} + C_3[\theta^6_{\sigma\varepsilon M} + W_0^2\theta^2_{\sigma\varepsilon M}].$$

Thus, from Lemma 2.3(ii), it follows from (2.23) that

$$\iint_{\Omega_T} (\partial_\theta \mathcal{F}_{\sigma\varepsilon M})^2 + \frac{\kappa^2}{2}\iint_{\Omega_T} [\theta_{\sigma\varepsilon M}]^2_{xx} \leq C_3.$$

Now, we prove item (iii). Defining, $H_{\sigma\varepsilon M} = \partial_c \mathcal{F}_{\sigma\varepsilon M} - \kappa_c[c_{\sigma\varepsilon M}]_{xx}$, since $[c_{\sigma\varepsilon M}]_{x|S_T} = 0$, we have

$$\iint_{\Omega_T} H_{\sigma\varepsilon M} = \iint_{\Omega_T} \partial_c \mathcal{F}_{\sigma\varepsilon M},$$

and from Lemma 2.3(iii),

$$\iint_{\Omega_T} [H_{\sigma\varepsilon M}]^2_x \leq C_1.$$

Using the definition of $\mathcal{F}_{\sigma\varepsilon M}$, given in (2.10), and an integration by parts, we obtain

$$\iint_{\Omega_T} H^2_{\sigma\varepsilon M} = \iint_{\Omega_T} (\partial_c \mathcal{F}_{\sigma\varepsilon M})^2 + 2\kappa_c\varepsilon \iint_{\Omega_T} [F''_\sigma(c_{\sigma\varepsilon M}) + F''_\sigma(1 - c_{\sigma\varepsilon M})][c_{\sigma\varepsilon M}]^2_x$$
$$- 2\kappa_c L \iint_{\Omega_T} (f'(c_{\sigma\varepsilon M}) + h'_1(c_{\sigma\varepsilon M})h_2(M;\theta_{\sigma\varepsilon M}))[c_{\sigma\varepsilon M}]_{xx} + \kappa_c^2 \iint_{\Omega_T} [c_{\sigma\varepsilon M}]^2_{xx}.$$

On the other hand, we can write

$$\iint_{\Omega_T} H^2_{\sigma\varepsilon M} = \iint_{\Omega_T} [H_{\sigma\varepsilon M} - \overline{H_{\sigma\varepsilon M}}]^2 + \iint_{\Omega_T} \overline{H_{\sigma\varepsilon M}}^2 \leq C_P \iint_{\Omega_T} [H_{\sigma\varepsilon M}]^2_x + \iint_{\Omega_T} (\partial_c \mathcal{F}_{\sigma\varepsilon M})^2$$

where C_P denotes the Poincaré constant. From these two last results, item (iii) follows recalling that $[F''_\sigma(c_{\sigma\varepsilon M}) + F''_\sigma(1 - c_{\sigma\varepsilon M})] \geq 0$ and using (2.11), (2.12), (2.13) and Lemma 2.3(ii).

Finally, recalling that for each σ, $F'_\sigma(s)$ is bounded in $\mathbf{R}$, using again the definition of f and h_M and Lemma 2.3(ii), we obtain

$$\begin{aligned}\|\partial_c \mathcal{F}_{\sigma\varepsilon M}\|^2_{L^2(\Omega_T)} &\leq C \iint_{\Omega_T} \{[f'(c_{\sigma\varepsilon M})]^2 + [h'_1(c_{\sigma\varepsilon M})]^2 [h_2(M;\theta_{\sigma\varepsilon M})]^2 \\ &\quad + \varepsilon^2 [F'_\sigma(c_{\sigma\varepsilon M}) - F'_\sigma(1 - c_{\sigma\varepsilon M})]\} \\ &\leq C\{Z_0^2[|\Omega_T| + \|\theta_{\sigma\varepsilon M}\|^4_{L^4}] + C(\sigma)\} \leq C'_3(\sigma).\end{aligned}$$

An analogous argument shows that $\|[\partial_c \mathcal{F}_{\sigma\varepsilon M}]_x\|^2_{L^2(\Omega_T)}$ is also bounded by a constant which depends only on σ. Thus, we have proved the item (i).

We can now state the following result.

PROPOSITION 2.2 For σ (sufficiently small), there exists a pair $(c_{\sigma\varepsilon}, \theta_{\sigma\varepsilon})$ such that:

(i). $c_{\sigma\varepsilon} \in L^\infty(0, T, H^1(\Omega)) \cap L^2(0, T, H^3(\Omega))$

(ii). $\theta_{\sigma\varepsilon} \in L^\infty(0, T, H^1(\Omega)) \cap L^2(0, T, H^2(\Omega))$

(iii). $\partial_t c_{\sigma\varepsilon} \in L^2(0, T, [H^1(\Omega)]')$, $\quad \partial_t \theta_{\sigma\varepsilon} \in L^2(\Omega_T)$

(iv). $\partial_c \mathcal{F}_{\sigma\varepsilon}(c_{\sigma\varepsilon}, \theta_{\sigma\varepsilon})$, $\partial_\theta \mathcal{F}_{\sigma\varepsilon}(c_{\sigma\varepsilon}, \theta_{\sigma\varepsilon}) \in L^2(\Omega_T)$

(v). $c_{\sigma\varepsilon}(0) = c_0$ and $\theta_{\sigma\varepsilon}(0) = \theta_0$ in $L^2(\Omega)$

(vi). $[c_{\sigma\varepsilon}]_{x|_{S_T}} = [\theta_{\sigma\varepsilon}]_{x|_{S_T}} = 0$ in $L^2(S_T)$

(vii). $(c_{\sigma\varepsilon}, \theta_{\sigma\varepsilon})$ solves the perturbed system (2.15) in the following sense:

$$\int_0^T \langle \partial_t c_{\sigma\varepsilon}, \phi \rangle = -\iint_{\Omega_T} D[\partial_c \mathcal{F}_{\sigma\varepsilon}(c_{\sigma\varepsilon}, \theta_{\sigma\varepsilon}) - \kappa_c (c_{\sigma\varepsilon})_{xx}]_x \phi_x \tag{2.24}$$

for all $\phi \in L^2(0, T, H^1(\Omega))$, and

$$\iint_{\Omega_T} \partial_t \theta_{\sigma\varepsilon} \psi = -\iint_{\Omega_T} L(\partial_\theta \mathcal{F}_{\sigma\varepsilon}(c_{\sigma\varepsilon}, \theta_{\sigma\varepsilon}) - \kappa(\theta_{\sigma\varepsilon})_{xx})\psi \tag{2.25}$$

for all $\psi \in L^2(\Omega_T)$, and $\mathcal{F}_{\sigma\varepsilon}$ is given by

$$\mathcal{F}_{\sigma\varepsilon}(c, \theta) = f(c) + \frac{\delta}{4}\theta^4 + h_1(c)\theta^2 + \varepsilon[F_\sigma(c) + F_\sigma(1 - c)].$$

Proof. First, let us observe that from Lemma 2.3(iii) and Lemma 2.4(i), the norm of $[c_{\sigma\varepsilon M}]_{xxx}$ in $L^2(\Omega_T)$ is bounded by a constant which does not depend on M. This fact, the estimates of Lemmas 2.3 and 2.4 together with a compactness argument imply that there exists a subsequence (still denoted by $\{(c_{\sigma\varepsilon M}, \theta_{\sigma\varepsilon M})\}$) that satisfies (as M goes to infinity)

$$\begin{array}{llll}
c_{\sigma\varepsilon M},\ \theta_{\sigma\varepsilon M} & \text{converge weakly-* to} & c_{\sigma\varepsilon}, \theta_{\sigma\varepsilon} & \text{in} \ L^\infty(0,T,H^1(\Omega)), \\
c_{\sigma\varepsilon M}, & \text{converges weakly to} & c_{\sigma\varepsilon} & \text{in} \ L^2(0,T,H^3(\Omega)), \\
\theta_{\sigma\varepsilon M}, & \text{converges weakly to} & \theta_{\sigma\varepsilon} & \text{in} \ L^2(0,T,H^2(\Omega)), \\
\partial_t c_{\sigma\varepsilon M}, & \text{converges weakly to} & \partial_t c_{\sigma\varepsilon} & \text{in} \ L^2(0,T,[H^1(\Omega)]'), \\
\partial_t \theta_{\sigma\varepsilon M}, & \text{converges weakly to} & \partial_t \theta_{\sigma\varepsilon} & \text{in} \ L^2(\Omega_T) \\
c_{\sigma\varepsilon M},\ \theta_{\sigma\varepsilon M} & \text{converge to} & c_{\sigma\varepsilon}, \theta_{\sigma\varepsilon} & \text{in} \ L^2(\Omega_T).
\end{array}$$

By recalling Lemmas 2.3 and 2.4, items (i)–(iii) now follow. Now, items (i) and (ii) of Lemma 2.4 imply that

$$\begin{array}{llll}
\partial_c \mathcal{F}_{\sigma\varepsilon M}(c_{\sigma\varepsilon M}, \theta_{\sigma\varepsilon M}) & \text{converges weakly to} & \mathcal{G} & \text{in} \ L^2(\Omega_T), \\
\partial_\theta \mathcal{F}_{\sigma\varepsilon M}(c_{\sigma\varepsilon M}, \theta_{\sigma\varepsilon M}) & \text{converges weakly to} & \mathcal{H} & \text{in} \ L^2(\Omega_T).
\end{array}$$

Since the strong convergence of the sequence $(c_{\sigma\varepsilon M})$ implies that (at least for a subsequence) $\partial_c \mathcal{F}_{\sigma\varepsilon M}(c_{\sigma\varepsilon M}, \theta_{\sigma\varepsilon M})$ converges pointwise in Ω_T, it follows from Lemma 1.3 from Lions [7], p. 12, that $\mathcal{G} = \partial_c \mathcal{F}_{\sigma\varepsilon}(c_{\sigma\varepsilon}, \theta_{\sigma\varepsilon})$. Similarly, we have $\mathcal{H} = \partial_\theta \mathcal{F}_{\sigma\varepsilon}(c_{\sigma\varepsilon}, \theta_{\sigma\varepsilon})$. Thus item (iv) is proved.

Item (v) is straightforward. Now, by compactness we have that

$$\begin{array}{lllll}
c_{\sigma\varepsilon M} & \text{converges to} & c_{\sigma\varepsilon} & \text{in} \ L^2(0,T,H^{2-\lambda}(\Omega)), & \lambda > 0, \\
\theta_{\sigma\varepsilon M} & \text{converges to} & \theta_{\sigma\varepsilon} & \text{in} \ L^2(0,T,H^{2-\lambda}(\Omega)), & \lambda > 0,
\end{array}$$

which imply item (vi).

To prove item (vii), by using the previous convergences, we pass to the limit as M goes to infinity in the equations (2.17) and (2.18).

2.5 Limit as $\sigma \to 0^+$

In this section we obtain some a priori estimates that allow taking the limit in the parameter σ.

First, let us note that (2.24) implies that the mean value of $c_{\sigma\varepsilon}$ in Ω is given by

$$\overline{c_{\sigma\varepsilon}(t)} = \overline{c_0} \in (0,1), \tag{2.26}$$

We start with the following Lemma.

LEMMA 2.5 There exists a constant C_1 independent of ε and σ (sufficiently small) such that

(i). $||c_{\sigma\varepsilon}||_{L^\infty(0,T,H^1(\Omega))} \leq C_1$

(ii). $||\theta_{\sigma\varepsilon}||_{L^\infty(0,T,H^1(\Omega))} \leq C_1$

(iii). $||[\partial_c\mathcal{F}_{\sigma\varepsilon} - \kappa_c(c_{\sigma\varepsilon})_{xx}]_x||_{L^2(\Omega_T)} \leq C_1$

(iv). $||\partial_\theta\mathcal{F}_{\sigma\varepsilon} - \kappa(\theta_{\sigma\varepsilon})_{xx}||_{L^2(\Omega_T)} \leq C_1$

(v). $||\partial_t c_{\sigma\varepsilon}||_{L^2(0,T,[H^1(\Omega)]')} \leq C_1$

(vi). $||\partial_t\theta_{\sigma\varepsilon}||_{L^2(\Omega_T)} \leq C_1$

(vii). $||\mathcal{F}_{\sigma\varepsilon}(c_{\sigma\varepsilon},\theta_{\sigma\varepsilon})||_{L^\infty(0,T,L^1(\Omega))} \leq C_1$

Proof. Let us observe that in the proof of Proposition 2.2, we have identified the weak limits, when M goes to infinity, of the sequences $\partial_c\mathcal{F}_{\sigma\varepsilon M}$ and $\partial_\theta\mathcal{F}_{\sigma\varepsilon M}$ as $\partial_c\mathcal{F}_{\sigma\varepsilon}$ and $\partial_\theta\mathcal{F}_{\sigma\varepsilon}$, respectively. Thus, by taking the inferior limit as M goes to infinity, of estimate (2.22), we obtain

$$\begin{aligned}&\frac{\kappa_c}{2}||(c_{\sigma\varepsilon})_x||^2_{L^\infty(0,T,L^2(\Omega))} + \frac{\kappa}{2}||(\theta_{\sigma\varepsilon})_x||^2_{L^\infty(0,T,L^2(\Omega))}\\ &+ D||[\partial_c\mathcal{F}_{\sigma\varepsilon} - \kappa_c(c_{\sigma\varepsilon})_{xx}]_x||^2_{L^2(\Omega_T)} + L||\partial_\theta\mathcal{F}_{\sigma\varepsilon} - \kappa(\theta_{\sigma\varepsilon})_{xx}||^2_{L^2(\Omega_T)} \leq C_1.\end{aligned} \tag{2.27}$$

The items (iii) and (iv) follow from (2.27). Using (2.27), Poincaré's inequality and (2.26), we obtain item (i). To prove items (ii), (v) and (vi), we just take the inferior limit of items (ii), (v) and (vi) of Lemma 2.3. Finally, the estimates and convergences obtained in Section 2.4, (2.11), (2.12), (2.13), the choice of F_σ and item (vii) of Lemma 2.3 yield item (vii).

As Passo et al. [3], by arguing in a standard way (see Bernis and Friedman [1] for a proof, p. 183), we obtain

Corolary 2.1 There exists a constant C_2 independent of ε and σ (sufficiently small) such that

$$||c_{\sigma\varepsilon}||_{C^{0,\frac{1}{2},\frac{1}{8}}(\mathrm{cl}\,\Omega_T)} \leq C_2 \qquad \text{and} \qquad ||\theta_{\sigma\varepsilon}||_{C^{0,\frac{1}{2},\frac{1}{8}}(\mathrm{cl}\,\Omega_T)} \leq C_2$$

By Corollary 2.1, we can extract a subsequence (still denoted by $(c_{\sigma\varepsilon}, \theta_{\sigma\varepsilon})$) such that

$$\begin{aligned} &(c_{\sigma\varepsilon}, \theta_{\sigma\varepsilon}) \text{ converges uniformly to } (c_\varepsilon, \theta_\varepsilon) \text{ in } \mathrm{cl}\,\Omega_T \text{ as } \sigma \text{ goes to zero,} \\ &c_\varepsilon \in C^{0,\frac{1}{2},\frac{1}{8}}(\mathrm{cl}\,\Omega_T) \qquad \text{and} \qquad \theta_\varepsilon \in C^{0,\frac{1}{2},\frac{1}{8}}(\mathrm{cl}\,\Omega_T). \end{aligned}$$

We now demonstrate that the limit c_ε lies within the interval

$$I = \{c \in \mathbb{R}, 0 < c < 1\}.$$

Lemma 2.6 $|\Omega_T \setminus \mathcal{B}(c_\varepsilon)| = 0$ with $\mathcal{B}(c) = \{(x,t) \in \mathrm{cl}\,\Omega_T,\ c(x,t) \in I\}$.

Proof. Arguing as Passo et al. [3], let N denote the operator defined as minus the inverse of the Laplacian with zero Neumann boundary conditions. That is, given $f \in [H^1(\Omega)]'_{null} = \{f \in [H^1(\Omega)]',\ \langle f, 1\rangle = 0\}$, we define $Nf \in H^1(\Omega)$ as the unique solution of

$$\int_\Omega (Nf)'\psi' = \langle f, \psi\rangle, \quad \forall \psi \in H^1(\Omega) \qquad \text{and} \qquad \int_\Omega Nf = 0.$$

By (2.26) and Lemma 2.5(i), $N(c_{\sigma\varepsilon} - \overline{c_{\sigma\varepsilon}})$ is well defined. Choosing $\phi = N(c_{\sigma\varepsilon} - \overline{c_{\sigma\varepsilon}})$ as a test function in the equation (2.24), we have

$$\begin{aligned} \int_0^T \langle \partial_t c_{\sigma\varepsilon}, N(c_{\sigma\varepsilon} - \overline{c_{\sigma\varepsilon}})\rangle dt &= -\iint_{\Omega_T} D[\partial_c \mathcal{F}_{\sigma\varepsilon} - \kappa_c (c_{\sigma\varepsilon})_{xx}]_x [N(c_{\sigma\varepsilon} - \overline{c_{\sigma\varepsilon}})]_x \\ &= -\iint_{\Omega_T} D(c_{\sigma\varepsilon} - \overline{c_{\sigma\varepsilon}})\partial_c \mathcal{F}_{\sigma\varepsilon}(c_{\sigma\varepsilon}, \theta_{\sigma\varepsilon}) - D\kappa_c \iint_{\Omega_T} [(c_{\sigma\varepsilon})_x]^2 \end{aligned}$$

Now, estimates in Lemma 2.5 and the definition of N imply

$$\iint_{\Omega_T} (c_{\sigma\varepsilon} - \overline{c_{\sigma\varepsilon}})\partial_c \mathcal{F}_{\sigma\varepsilon}(c_{\sigma\varepsilon}, \theta_{\sigma\varepsilon}) \leq C_4. \tag{2.28}$$

We observe that the following identity holds for any $m \in \mathbf{R}$,

$$\begin{aligned} (c-m)\partial_c \mathcal{F}_{\sigma\varepsilon}(c,\theta) &= (c-m)[f'(c) + h_1'(c)\theta^2 + \varepsilon(F_\sigma'(c) - F_\sigma'(1-c))] \\ &= \varepsilon\{c[F_\sigma'(c) - 1] + (1-c)[F_\sigma'(1-c) - 1] + 2\} \\ &\quad + (c-m)[f'(c) + h_1'(c)\theta^2] - \varepsilon - \varepsilon m F_\sigma'(c) - \varepsilon(1-m)F_\sigma'(1-c) \end{aligned} \tag{2.29}$$

We observe that the terms inside the braces are bounded from below since for any $\sigma \in (0, 1/e)$, we have

$$
\begin{gathered}
-1/e \leq \sigma \ln \sigma \leq s[F'_\sigma(s) - 1] \leq 0, \quad s \leq \sigma, \\
-1/e \leq s \ln s = s[F'_\sigma(s) - 1] \leq 0, \quad \sigma \leq s \leq 1 - \sigma, \\
-2 \leq s[F'_\sigma(s) - 1] \leq 0, \quad 1 - \sigma \leq s \leq 2, \\
0 = s[F'_\sigma(s) - 1], \quad s \geq 2.
\end{gathered}
$$

We now recall that the mean value of $c_{\sigma\varepsilon}$ in Ω is conserved and is equal to $\overline{c_0}$ which belongs to the interval $(0, 1)$. Thus, since f', h'_1 are uniformly bounded, using the estimates in Lemma 2.5, by setting $m = \overline{c_{\sigma\varepsilon}} = \overline{c_0}$ in (2.29), it follows from (2.28) that

$$
\begin{aligned}
-\varepsilon p \iint_{\Omega_T} &[F'_\sigma(c_{\sigma\varepsilon}) + F'_\sigma(1 - c_{\sigma\varepsilon})] - \varepsilon \iint_{\Omega_T} [(\overline{c_0} - p)F'_\sigma(c_{\sigma\varepsilon}) + (1 - \overline{c_0} - p)F'_\sigma(1 - c_{\sigma\varepsilon})] \\
&= -\varepsilon \iint_{\Omega_T} [(\overline{c_0} F'_\sigma(c_{\sigma\varepsilon}) + (1 - \overline{c_0})F'_\sigma(1 - c_{\sigma\varepsilon})] + \leq C_4.
\end{aligned}
$$

where $p = \min\{\overline{c_0}, 1 - \overline{c_0}\}$. Noting that $F'_\sigma \leq 1$, we obtain

$$
-\varepsilon \iint_{\Omega_T} [F'_\sigma(c_{\sigma\varepsilon}) + F'_\sigma(1 - c_{\sigma\varepsilon})] \leq C_4 \tag{2.30}
$$

To complete the proof, suppose by contradiction that the set $\Omega_T \setminus \mathcal{B}(c_\varepsilon)$ has a positive measure. Now suppose that

$$
A = \{(x, t) \in \Omega_T, \ c_\varepsilon \leq 0\}
$$

has positive measure. Since $F'_\sigma \leq 1$, the estimate (2.30) gives

$$
-\varepsilon \iint_A F'_\sigma(c_{\sigma\varepsilon}) \leq C_4.
$$

Note, however, that the uniform convergence of $c_{\sigma\varepsilon}$ implies that

$$
\forall \lambda > 0, \ \exists \sigma_\lambda, \quad c_{\sigma\varepsilon} \leq \lambda, \quad \forall (x, t) \in A, \ \sigma < \sigma_\lambda
$$

therefore, due to the convexity of F_σ, we have $F'_\sigma(c_{\sigma\varepsilon}) \leq F'_\sigma(\lambda)$. hence

$$
-\varepsilon |A| (\ln \lambda + 1) = -\varepsilon \iint_A F'_\sigma(\lambda) \leq -\varepsilon \iint_A F'_\sigma(c_{\sigma\varepsilon}) \leq C_4
$$

which leads to a contradiction for λ sufficiently small. The same argument shows that $B = \{(x,t) \in \Omega_T,\ c_\varepsilon \geq 1\}$ has zero measure.

In the next lemma we derive additional estimates which allow us to pass to the limit as σ tends to zero. Its proof follows directly from the estimates of Lemma 2.5.

LEMMA 2.7 There exists a constant C_3 which is independent of ε and σ (sufficiently small) such that

(i). $||\partial_\theta \mathcal{F}_{\sigma\varepsilon}||_{L^2(\Omega_T)} \leq C_3$,

(ii). $||[c_{\sigma\varepsilon}]_{xx}||_{L^2(\Omega_T)} \leq C_3$,

(iii). $||[\theta_{\sigma\varepsilon}]_{xx}||_{L^2(\Omega_T)} \leq C_3$,

To pass to the limit as σ goes to zero, we need an estimate of $\partial_c \mathcal{F}_{\sigma\varepsilon}$ that is independent of σ. We cannot repeat the argument that we used in Lemma 2.4 because there we obtained a constant that depends on σ. The desired estimate will be obtained by using the next lemma, presented by Copetti and Elliott [2], p. 48, and by Elliott and Luckhaus [5], p. 23.

LEMMA 2.8 Let $v \in L^1(\Omega)$ such that there exist positive constants δ_1 and δ_1' satisfying

$$8\delta_1 < \frac{1}{|\Omega|} \int_\Omega v dx < 1 - 8\delta_1,$$

$$\frac{1}{|\Omega|} \int_\Omega ([v-1]_+ + [-v]_+)\, dx < \delta_1'. \tag{2.31}$$

If $16\delta_1' < \delta_1^2$ then

$$|\Omega_{\delta_1}^+| = |\{x \in \Omega, \quad v(x) > 1 - 2\delta_1\}| < (1-\delta_1)\,|\Omega|$$

and

$$|\Omega_{\delta_1}^-| = |\{x \in \Omega, \quad v(x) < 2\delta_1\}| < (1-\delta_1)\,|\Omega|.$$

Our task is now to verify the hypothesis of this last lemma for the functions $c_{\sigma\varepsilon}$. To obtain (2.31), we note that items (ii) and (vii) of Lemma 2.5, (2.11) and (2.12) imply that, for almost every $t \in [0,T]$,

$$\varepsilon \int_\Omega [F_\sigma(c_{\sigma\varepsilon}) + F_\sigma(1-c_{\sigma\varepsilon})]dx \leq C_1 + \left\| f(c_{\sigma\varepsilon}) + \delta\theta_{\sigma\varepsilon}^4/4 + h_1(c_{\sigma\varepsilon})\theta_{\sigma\varepsilon}^2 \right\|_{L^\infty(0,T,L^1(\Omega))} \leq C.$$

Now, since $F_\sigma(s) \geq -1/e$, we have

$$\begin{aligned}\varepsilon \int_\Omega F_\sigma(c_{\sigma\varepsilon})dx &= \varepsilon \int_{\{c_{\sigma\varepsilon}\geq 0\}} F_\sigma(c_{\sigma\varepsilon})dx + \varepsilon \int_{\{c_{\sigma\varepsilon}<0\}} F_\sigma(c_{\sigma\varepsilon})dx \\ &\geq -\varepsilon|\Omega|e^{-1} + \varepsilon|\ln\sigma| \int_\Omega [-c_{\sigma\varepsilon}(\cdot,t)]_+dx - \varepsilon\sigma[|\ln\sigma| + 2\sigma]|\Omega| - \varepsilon\sigma\|c_{\sigma\varepsilon}(t)\|_{L^2(\Omega)}|\Omega|^{1/2}\end{aligned}$$

In the same way, we have

$$\begin{aligned}\varepsilon \int_\Omega F_\sigma(1-c_{\sigma\varepsilon})dx \geq& -\varepsilon|\Omega|e^{-1} + \varepsilon|\ln\sigma| \int_\Omega [c_{\sigma\varepsilon}(\cdot,t)-1]_+dx \\ &- \varepsilon\sigma[|\ln\sigma| + 2\sigma + 1]|\Omega| - \varepsilon\sigma\|c_{\sigma\varepsilon}(t)\|_{L^2(\Omega)}|\Omega|^{1/2}\end{aligned}$$

Thus, using the above estimates and Lemma 2.5(i), we obtain

$$\int_\Omega [c_{\sigma\varepsilon}(\cdot,t)-1]_+dx + \int_\Omega [-c_{\sigma\varepsilon}(\cdot,t)]_+dx \leq \frac{C}{\varepsilon|\ln\sigma|}$$

The equation (2.26) says that the mean value of $c_{\sigma\varepsilon}$ is equal to $\overline{c_0}$ which belongs to $(0,1)$. Thus there exists $\delta_1 > 0$, such that $\delta_1 < \overline{c_0} < 1-\delta_1$. Using Lemma 2.8, for σ sufficiently small, we have for almost every $t \in [0,T]$

$$\begin{aligned}|\Omega_{\sigma\delta_1}^+| &= \{x \in \Omega, \quad c_{\sigma\varepsilon}(x,t) > 1-2\delta_1\} < (1-\delta_1)\,|\Omega|, \\ |\Omega_{\sigma\delta_1}^-| &= \{x \in \Omega, \quad c_{\sigma\varepsilon}(x,t) < 2\delta_1\} < (1-\delta_1)\,|\Omega|.\end{aligned} \tag{2.32}$$

We are now in position to estimate $\partial_c\mathcal{F}_{\sigma\varepsilon}(c_{\sigma\varepsilon},\theta_{\sigma\varepsilon})$.

LEMMA 2.9 There exists a constant C_4 which is independent of ε and σ (sufficiently small) such that

$$\|\partial_c\mathcal{F}_{\sigma\varepsilon}(c_{\sigma\varepsilon},\theta_{\sigma\varepsilon})\|_{L^2(\Omega_T)} \leq C_4.$$

Proof. First, let us recall that

$$\partial_c \mathcal{F}_{\sigma\varepsilon} = f'(c_{\sigma\varepsilon}) + h_1'(c_{\sigma\varepsilon})\theta_{\sigma\varepsilon}^2 + \varepsilon[F_\sigma'(c_{\sigma\varepsilon}) - F_\sigma'(1-c_{\sigma\varepsilon})].$$

In view of Lemma 2.5(ii), (2.11) and (2.12), the main difficulty in the argument is to obtain the desired estimate is to obtain a bound for the norm of $\varepsilon[F_\sigma'(c_{\sigma\varepsilon}) - F_\sigma'(1-c_{\sigma\varepsilon})]$ in $L^2(\Omega_T)$. Arguing as Copetti and Elliott [2], we obtain this bound by using the next equality

$$\begin{aligned} &\left\|\varepsilon[F_\sigma'(c_{\sigma\varepsilon}) - F_\sigma'(1-c_{\sigma\varepsilon})] - \overline{\varepsilon[F_\sigma'(c_{\sigma\varepsilon}) - F_\sigma'(1-c_{\sigma\varepsilon})]}\right\|^2_{L^2(\Omega_T)} \\ &= \|\varepsilon[F_\sigma'(c_{\sigma\varepsilon}) - F_\sigma'(1-c_{\sigma\varepsilon})]\|^2_{L^2(\Omega_T)} - \iint_{\Omega_T} \left(\overline{\varepsilon[F_\sigma'(c_{\sigma\varepsilon}) - F_\sigma'(1-c_{\sigma\varepsilon})]}\right)^2 \end{aligned} \tag{2.33}$$

and estimating the term at the left hand side and the last term at the right hand side of the above equation.

Let us note that using Poincaré inequality and Lemma 2.5(iii), we obtain

$$\|\partial_c \mathcal{F}_{\sigma\varepsilon}(c_{\sigma\varepsilon}, \theta_{\sigma\varepsilon}) - \kappa_c(c_{\sigma\varepsilon})_{xx} - \overline{\partial_c \mathcal{F}_{\sigma\varepsilon}(c_{\sigma\varepsilon}, \theta_{\sigma\varepsilon}) - \kappa_c(c_{\sigma\varepsilon})_{xx}}\|_{L^2(\Omega_T)} \le C_1.$$

Recalling that $c_{x|S_T} = 0$, we have

$$\overline{\partial_c \mathcal{F}_{\sigma\varepsilon}(c_{\sigma\varepsilon}, \theta_{\sigma\varepsilon}) - \kappa_c(c_{\sigma\varepsilon})_{xx}} = \overline{f'(c_{\sigma\varepsilon}) + h_1'(c_{\sigma\varepsilon})\theta_{\sigma\varepsilon}^2 + \varepsilon[F_\sigma'(c_{\sigma\varepsilon}) - F_\sigma'(1-c_{\sigma\varepsilon})]}.$$

Thus, using the estimates for $(c_{\sigma\varepsilon})_{xx}$ in Lemma 2.7(ii) and for $\theta_{\sigma\varepsilon}$ in Lemma 2.5(ii) together (2.11) and (2.12), we obtain

$$\|\varepsilon[F_\sigma'(c_{\sigma\varepsilon}) - F_\sigma'(1-c_{\sigma\varepsilon})] - \overline{\varepsilon[F_\sigma'(c_{\sigma\varepsilon}) - F_\sigma'(1-c_{\sigma\varepsilon})]}\|_{L^2(\Omega_T)} \le \widetilde{C}_1 \tag{2.34}$$

We now use the monotonicity of $F_\sigma'(s) - F_\sigma'(1-s)$ and (2.32) to obtain for almost every $t \in [0,T]$:

$$\begin{aligned} &\overline{\varepsilon[F_\sigma'(c_{\sigma\varepsilon}) - F_\sigma'(1-c_{\sigma\varepsilon})]} \\ &= \varepsilon|\Omega|^{-1} \int_{\Omega^+_{\sigma\delta_1}} [F_\sigma'(c_{\sigma\varepsilon}) - F_\sigma'(1-c_{\sigma\varepsilon})] + \varepsilon|\Omega|^{-1} \int_{[\Omega^+_{\sigma\delta_1}]^c} [F_\sigma'(c_{\sigma\varepsilon}) - F_\sigma'(1-c_{\sigma\varepsilon})] \\ &\le (1-\delta_1)^{1/2} |\Omega|^{-1/2} \|\varepsilon[F_\sigma'(c_{\sigma\varepsilon}) - F_\sigma'(1-c_{\sigma\varepsilon})]\|_{L^2(\Omega)} + \varepsilon\left[F_\sigma'(1-2\delta_1) - F_\sigma'(2\delta_1)\right]. \end{aligned}$$

In the same way, observing that $F'_\sigma(2\delta_1) - F'_\sigma(1-2\delta_1) < 0$, we have

$$\overline{\varepsilon[F'_\sigma(c_{\sigma\varepsilon}) - F'_\sigma(1-c_{\sigma\varepsilon})]} \geq -(1-\delta_1)^{1/2}\,|\Omega|^{-1/2}\|\varepsilon[F'_\sigma(c_{\sigma\varepsilon}) - F'_\sigma(1-c_{\sigma\varepsilon})]\|_{L^2(\Omega)} + \varepsilon\left[F'_\sigma(2\delta_1) - F'_\sigma(1-2\delta_1)\right].$$

Therefore, by using that $(a+b)^2 \leq a^2\left(1+\frac{1}{\delta_1}\right) + b^2(1+\delta_1)$, we have

$$\left(\overline{\varepsilon[F'_\sigma(c_{\sigma\varepsilon}) - F'_\sigma(1-c_{\sigma\varepsilon})]}\right)^2 \leq \varepsilon\left(1+\frac{1}{\delta_1}\right)\left[F'_\sigma(1-2\delta_1) - F'_\sigma(2\delta_1)\right]^2 + (1-\delta_1^2)\frac{1}{|\Omega|}\|\varepsilon[F'_\sigma(c_{\sigma\varepsilon}) - F'_\sigma(1-c_{\sigma\varepsilon})]\|^2_{L^2(\Omega)}.$$

Multiplying the above estimate by $|\Omega|$, integrating it in t and using (2.33) and (2.34), it results that for σ sufficiently small, we have

$$\begin{aligned}\delta_1^2\|\varepsilon[F'_\sigma(c_{\sigma\varepsilon}) - F'_\sigma(1-c_{\sigma\varepsilon})]\|^2_{L^2(\Omega_T)} &\leq \varepsilon|\Omega_T|\left(1+\frac{1}{\delta_1}\right)\left[F'_\sigma(2\delta_1) - F'_\sigma(1-2\delta_1)\right]^2 \\ &+ \left\|\varepsilon[F'_\sigma(c_{\sigma\varepsilon}) - F'_\sigma(1-c_{\sigma\varepsilon})] - \overline{\varepsilon[F'_\sigma(c_{\sigma\varepsilon}) - F'_\sigma(1-c_{\sigma\varepsilon})]}\right\|^2_{L^2(\Omega_T)} \\ &\leq \varepsilon|\Omega_T|\left(1+\frac{1}{\delta_1}\right)\left[F'(2\delta_1) - F'(1-2\delta_1)\right]^2 + \widetilde{C}_1 \leq \widetilde{C}_2.\end{aligned}$$

We define

$$w_{\sigma\varepsilon} = D(\partial_c\mathcal{F}_{\sigma\varepsilon}(c_{\sigma\varepsilon},\theta_{\sigma\varepsilon}) - \kappa_c[c_{\sigma\varepsilon}]_{xx}),$$

the estimates in Lemmas 2.5, 2.7 and 2.9 and Lemma 2.6 imply

$$\begin{aligned} w_{\sigma\varepsilon} \quad &\text{converge weakly to} \quad w_\varepsilon \quad \text{in} \quad L^2(0,T,H^1(\Omega)), \\ &\text{where} \quad w_\varepsilon = D(\partial_c\mathcal{F}_\varepsilon(c_\varepsilon,\theta_\varepsilon) - \kappa_c[c_\varepsilon]_{xx}),\end{aligned}$$

and where $\mathcal{F}_\varepsilon$ is defined as in the next Proposition. Therefore, arguing as in Proposition 2.2, we can pass to the limit as σ goes to zero in equations (2.24) and (2.25) to obtain

PROPOSITION 2.3 There exists a triplet $(c_\varepsilon, w_\varepsilon, \theta_\varepsilon)$ such that:

(i). $c_\varepsilon, \theta_\varepsilon \in L^\infty(0,T,H^1(\Omega))$, (ii). $\partial_t c_\varepsilon \in L^2(0,T,[H^1(\Omega)]')$ and $\partial_t \theta_\varepsilon \in L^2(\Omega_T)$,

(iii). $[c_\varepsilon]_{xx}, [\theta_\varepsilon]_{xx} \in L^2(\Omega_T)$,

(iv). $|\Omega_T \setminus \mathcal{B}(c_\varepsilon)| = 0$,

(v). $\partial_c \mathcal{F}_\varepsilon(c_\varepsilon, \theta_\varepsilon), \partial_\theta \mathcal{F}_\varepsilon(c_\varepsilon, \theta_\varepsilon) \in L^2(\Omega_T)$,

(vi). $w_\varepsilon \in L^2(0,T,H^1(\Omega))$

(vii). $c_\varepsilon(0) = c_0(x), \quad \theta_{\varepsilon M}(0) = \theta_0(x)$

(viii). $[c_\varepsilon]_{x|S_T} = [\theta_{\varepsilon M}]_{x|S_T} = 0$ in $L^2(S_T)$

(ix). $(c_\varepsilon, w_\varepsilon, \theta_\varepsilon)$ satisfies

$$\int_0^T \langle \partial_t c_\varepsilon, \phi \rangle dt = -\iint_{\Omega_T} [w_\varepsilon]_x \phi_x, \quad \forall \phi \in L^2(0,T,H^1(\Omega))$$

$$w_\varepsilon = D[\partial_c \mathcal{F}_\varepsilon(c_\varepsilon, \theta_\varepsilon) - \kappa_c (c_\varepsilon)_{xx}] \tag{2.35}$$

$$\iint_{\Omega_T} \partial_t \theta_\varepsilon \psi = -\iint_{\Omega_T} L(\partial_\theta \mathcal{F}_\varepsilon(c_\varepsilon, \theta_\varepsilon) - \kappa(\theta_\varepsilon)_{xx})\psi, \quad \forall \psi \in L^2(\Omega_T)$$

where, since $c_\varepsilon \in (0,1)$ a.e in Ω_T,

$$\begin{aligned}\mathcal{F}_\varepsilon(c,\theta) = & -\frac{A}{2}(c-c_m)^2 + \frac{B}{4}(c-c_m)^4 + \frac{D_\alpha}{4}(c-c_\alpha)^4 + \frac{D_\beta}{4}(c-c_\beta)^4 \\ & + \frac{\delta}{4}\theta^4 - \frac{\gamma}{2}c^2\theta^2 + \varepsilon[F(c) + F(1-c)]\end{aligned}$$

with $F(s) = s \ln s$.

2.6 Limit as $\varepsilon \to 0^+$

In this section we finally prove Theorem 2.1. We start by observing that, as before, we have the mean value of c_ε in Ω given by

$$\overline{c_\varepsilon} = \overline{c_0} \in (0,1),$$

Since the estimates obtained for σ in Lemmas 2.5, 2.7 and 2.9 do not depend on ε, we have

LEMMA 2.10 There exists a constant C_1 independent of ε such that

(i). $\|c_\varepsilon\|_{L^\infty(0,T,H^1(\Omega))} \leq C_1$

(ii). $\|\theta_\varepsilon\|_{L^\infty(0,T,H^1(\Omega))} \leq C_1$

(iii). $\|(w_\varepsilon)_x\|_{L^2(\Omega_T)} \leq C_1$

(iv). $\|\partial_\theta \mathcal{F}_\varepsilon - \kappa(\theta_\varepsilon)_{xx}\|_{L^2(\Omega_T)} \leq C_1$

(v). $\|\partial_t c_\varepsilon\|_{L^2(0,T,[H^1(\Omega)]')} \leq C_1$

(vi). $\|\partial_t \theta_\varepsilon\|_{L^2(\Omega_T)} \leq C_1$

(vii). $\|\partial_c \mathcal{F}_\varepsilon(c_\varepsilon, \theta_\varepsilon)\|_{L^2(\Omega_T)} \leq C_1$,

(viii). $\|\partial_\theta \mathcal{F}_\varepsilon(c_\varepsilon, \theta_\varepsilon)\|_{L^2(\Omega_T)} \leq C_1$,

(ix). $\|[c_\varepsilon]_{xx}\|_{L^2(\Omega_T)} \leq C_1$,

(x). $\|[\theta_\varepsilon]_{xx}\|_{L^2(\Omega_T)} \leq C_1$

Now, we complete the proof of Theorem 2.1.
Proof in the case d = 1 and p = 1: We recall

$$\mathcal{F}(c,\theta) = -\frac{A}{2}(c-c_m)^2 + \frac{B}{4}(c-c_m)^4 + \frac{D_\alpha}{4}(c-c_\alpha)^4 + \frac{D_\beta}{4}(c-c_\beta)^4 - \frac{\gamma}{2}(c-c_\alpha)^2\theta^2 + \frac{\delta}{4}\theta^4$$

Then, we argue as Elliott and Luckhaus [5], p. 35. For this, let

$$\phi^\rho \in K^+ = \{\phi \in H^1(\Omega),\ 0 < \phi < 1\} \qquad \text{and} \qquad \rho < \phi^\rho < 1-\rho$$

for some small positive ρ. We have $[F'(\phi^\rho) - F'(1-\phi^\rho)] \in L^2(\Omega)$ because $\rho < \phi^\rho < 1-\rho$. Hence it follows from (2.35) that

$$\int_0^T \xi(t)(w_\varepsilon, \phi^\rho - c_\varepsilon)dt = D\int_0^T \xi(t)(\partial_c \mathcal{F}(c_\varepsilon,\theta_\varepsilon) + \varepsilon[F'(c_\varepsilon) - F'(1-c_\varepsilon)] - \kappa_c(c_\varepsilon)_{xx}, \phi^\rho - c_\varepsilon)dt.$$

Integrating by parts and rewriting, we obtain

$$\int_0^T \xi(t)\left\{\kappa_c(\nabla c_\varepsilon, \nabla\phi^\rho) - (w_\varepsilon - \partial_c\mathcal{F}(c_\varepsilon, \theta_\varepsilon), \phi^\rho - c_\varepsilon)\right\} dt$$

$$= \int_0^T \xi(t)\kappa_c(\nabla c_\varepsilon, \nabla c_\varepsilon)dt + \varepsilon\int_0^T \xi(t)([F'(\phi^\rho) - F'(1-\phi^\rho)] - [F'(c_\varepsilon) - F'(1-c_\varepsilon)], \phi^\rho - c_\varepsilon)dt$$

$$- \varepsilon\int_0^T \xi(t)([F'(\phi^\rho) - F'(1-\phi^\rho)], \phi^\rho - c_\varepsilon)dt.$$

By using the monotonicity of $F'(\cdot) - F'(1-\cdot)$ and the convergence properties of $(c_\varepsilon, w_\varepsilon, \theta_\varepsilon)$ we may pass to the limit and obtain for $\xi \in C[0,T]$, $\xi \geq 0$, that

$$\int_0^T \xi(t)\left\{\kappa_c(\nabla c, \nabla\phi^\rho) - (w - \partial_c\mathcal{F}(c, \theta), \phi^\rho - c)\right\} dt$$

$$= \lim_{\varepsilon\to 0}\int_0^T \xi(t)\left\{\kappa_c(\nabla c_\varepsilon, \nabla\phi^\rho) - (w - \partial_c\mathcal{F}(c_\varepsilon, \theta_\varepsilon), \phi^\rho - c_\varepsilon)\right\} dt$$

$$\geq \liminf_{\varepsilon\to 0}\int_0^T \xi(t)\kappa_c(\nabla c_\varepsilon, \nabla c_\varepsilon)dt - \lim_{\varepsilon\to 0}\varepsilon\int_0^T \xi(t)([F'(\phi^\rho) - F'(1-\phi^\rho)], \phi^\rho - c_\varepsilon)dt$$

$$\geq \int_0^T \xi(t)\kappa_c(\nabla c, \nabla c)dt.$$

Furthermore, since any $\phi \in K = \{\phi \in H^1(\Omega),\ \ 0 \leq \phi \leq 1, \overline{\eta} = \overline{c_0}\}$ can be approximated by $\phi^\rho \in K^+$, for small ρ with $\rho < \phi^\rho < 1-\rho$, we may pass to the limit as ρ goes to zero in the left hand side of the above inequality and obtain

$$\int_0^T \xi(t)\left\{\kappa_c(\nabla c, \nabla\phi - \nabla c) - (w - \partial_c\mathcal{F}(c, \theta), \phi - c)\right\} dt \geq 0 \qquad (2.36)$$

for $\xi \in C[0,T)$, $\xi \geq 0$, and $\phi \in K$.

Arguing as in the previous sections we also obtain

$$\int_0^T \langle\partial_t c, \phi\rangle dt = -\iint_{\Omega_T} w_x\phi_x, \quad \forall\phi \in L^2(0,T,H^1(\Omega)) \qquad (2.37)$$

and

$$\iint_{\Omega_T} \partial_t\theta\psi = -\iint_{\Omega_T} L(\partial_\theta\mathcal{F}(c,\theta) - \kappa\theta_{xx})\psi, \quad \forall\psi \in L^2(\Omega_T). \qquad (2.38)$$

Thus, for spatial dimension one and $p = 1$, Theorem 2.1 is a direct consequence of Lemma 2.10, (2.36), (2.37) and (2.38).

■

Now we argue that slight changes in the arguments previously presented prove the Theorem for higher spatial dimensions and $p > 1$.

Proof. Firstly, we discuss the case when the spatial dimension satisfies $d = 2, 3$. We start by remarking that, as observed by Passo et al. [3], Proposition 2.1 is valid for any dimension. Also, all of our previous arguments hold for dimensions $d = 2, 3$, except the result of Corollary 2.1, where the fact that dimension was one was essential. This result was only used, after Corollary 2.1, to extract an uniformly convergent subsequence that will be used in the proof of Lemma 2.6 to conclude that the measure of the set $\Omega_T \setminus \mathcal{B}(c_\varepsilon)$ is zero (where $\mathcal{B}(c) = \{(x,t) \in \mathrm{cl}\,\Omega_T,\ c(x,t) \in I\}$). Thus, to obtain the results in Lemma 2.6, in higher dimensions, we have to slightly modify our arguments. We just do that by means of a compacity argument used to extract a subsequence which converges almost uniformly in Ω_T. Thus, we just repeat the contradiction argument presented in the proof of Lemma 2.6 with the only difference that now we suppose by contradiction that there exists a subset of $\Omega_T \setminus \mathcal{B}(c_\varepsilon)$ that has positive measure and where the convergence is uniform.

Also, in higher dimensions, we use an argument of elliptic regularity of the Laplacian to obtain estimates in $L^2(0, T, H^2(\Omega))$ and in $L^2(0, T, H^3(\Omega))$.

Now we explain the necessary modifications when the number of crystallographic orientations is larger than one. In this case, the local free energy density is given by

$$\begin{aligned}\mathcal{F}(c,\theta) = &-\frac{A}{2}(c-c_m)^2 + \frac{B}{4}(c-c_m)^4 + \frac{D_\alpha}{4}(c-c_\alpha)^4 + \frac{D_\beta}{4}(c-c_\beta)^4 \\ &-\frac{\gamma}{2}\sum_{i=1}^{p}\left[(c-c_\alpha)^2\theta_i^2 + \frac{\delta}{4}\theta_i^4\right] + \sum_{i\neq j=1}^{p}\frac{\varepsilon_{ij}}{2}\theta_i^2\theta_j^2.\end{aligned}$$

Let us note that the introduction of the mixed terms depending only on the θ_i's (the last terms) will not change greatly the arguments presented in the case when p was equal to one. In the following we point out how our previous estimates can be extended for the case when p is larger than one.

The main feature of the perturbed systems in Section 2.3 is that their corresponding local free energy density have lower bounds that do not depend on the truncation parameter M. Since the extended local free energy just introduces non negative terms, we can define a similar truncation that maintains the same property, with such perturbed systems it is then possible to similarly establish Lemma 2.3.

As for Lemma 2.4, we treat the new terms by using the immersion of $H^1(\Omega)$ in $L^4(\Omega)$ and the estimates for the orientation field variables given in Lemma 2.3.

After we have extended the results of Lemmas 2.3 and 2.4, all the other lemmas are their direct consequence without any significative change due to the introduction of the new terms.

■

REMARK. We conclude with a brief remark about the solution obtained in Theorem 2.1. We note that in dimension one, using Corollary 2.1 we could extract a subsequence c_ε that converges uniformly in $\mathrm{cl}\,\Omega_T$ to c. Thus, the set $\{(x,t) \in \mathrm{cl}\,\Omega_T, 0 < c(x,t) < 1\}$ is an open set. With such information, when taking the limit as ε goes to zero, we could choose test functions with support in this set. Thus, when taking limit in (2.35), we will obtain an equality in (2.5) in the region where $0 < c(x,t) < 1$, and we can view the problem as a free boundary value problem. In this sense, we call our solution a generalized solution.

Bibliografia

[1] F. Bernis and A. Friedman. Higher order nonlinear degenerate parabolic equations. *Journal of Differential Equations*, 83:179–206, 1990.

[2] M. I. M. Copetti and Charles M. Elliott. Numerical analysis of the Cahn-Hilliard equation with a logarithmic free energy. *Numer. Math.*, 63:39–65, 1992.

[3] R. Dal Passo, L. Giacomelli, and A. Novick-Cohen. Existence for an Allen-Cahn/Cahn-Hilliard system with degenerate mobility. *Interfaces and Free Boundaries*, 1(2):199–226, 1999.

[4] C. Elliott and H. Garcke. On the Cahn-Hilliard equation with degenerate mobility. *SIAM Journal of Mathematical Analysis*, 27:404–423, 1996.

[5] Charles M. Elliott and Stefan Luckhaus. A generalised diffusion equation for phase separation of a multi-component mixture with interfacial free energy. Preprint 887, IMA (Minnesota), October 1991.

[6] Dan Fan, Long-Qing Chen, S.P. Chen, and Peter W. Voorhees. Phase field formulations for modelling the Ostwald ripening in two-phase systems. *Comp. Mater. Sci.*, 9:329–336, 1998.

[7] J.L. Lions. *Quelques méthodes de Résolution des Problèmes aux Limites non Linéaries.* Dunod, 1969.

Capítulo 3

Uma Solução Fraca de um Modelo para "Ostwald Ripening"

Resumo

Analisamos uma família de sistemas que acomplam uma equação do tipo Cahn-Hilliard a várias equações do tipo Allen-Cahn. Tais sistemas são análogos ao proposto por Fan, L.-Q. Chen, S. Chen e Voorhees para modelar o fenômeno "Ostwald ripening" em sistemas bifásicos. Para tal família, provamos a existência e unicidade de uma solução fraca.

A Weak Solution of a Model for Ostwald Ripening

Patrícia Nunes da Silva
nunes@ime.unicamp.br

José Luiz Boldrini
boldrini@ime.unicamp.br

Abstract

We analyze a family of systems consisting of a Cahn-Hilliard and several Allen-Cahn type equations. These systems are analogous to one proposed by Fan, L.-Q. Chen, S. Chen and Voorhees for modeling Ostwald ripening in two-phase systems. For such systems, we prove the existence and uniqueness of a weak solution.

3.1 Introduction

Ostwald ripening is a phenomenon observed in a wide variety of two-phase systems in which there is coarsening of one phase dispersed in the matrix of another. Because its practical importance, this process has been extensively studied in several degrees of generality. In particular for Ostwald ripening of anisotropic crystals, Fan et al. (1998) presented a model taking in consideration both the evolution of the compositional field and of the crystallographic orientations. In the work of Fan et al. (1998), there are also numerical experiments used to validate the model, but there is no rigorous mathematical analysis of the model.

Our objective in this paper is to do such mathematical analysis for a family of models of Ostwald ripening related to that presented by Fan et al. (1998). Such family is constituted of the following Cahn-Hilliard and Allen-Cahn equations:

$$\begin{cases} \partial_t c = \nabla \cdot \left[D\nabla \left(\partial_c \mathcal{F} - \kappa_c \Delta c \right) \right], & (x,t) \in \Omega_T \\ \partial_t \theta_i = -L_i \left(\partial_{\theta_i} \mathcal{F} - \kappa_i \Delta \theta_i \right), & (x,t) \in \Omega_T \\ \partial_{\mathrm{n}} c = \partial_{\mathrm{n}} \left(\partial_c \mathcal{F} - \kappa_c \Delta c \right) = \partial_{\mathrm{n}} \theta_i = 0, & (x,t) \in S_T \\ c(x,0) = c_0(x), \quad \theta_i(x,0) = \theta_{i0}(x), & x \in \Omega \end{cases} \tag{3.1}$$

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for $i = 1, \dots, p$.

Here, Ω is the physical region where the Ostwald process is occurring; $\Omega_T = \Omega \times (0, T)$; $S_T = \partial\Omega \times (0, T)$; $0 < T < +\infty$; $\mathbf{n}$ denotes the unitary exterior normal vector and $\partial_{\mathbf{n}}$ is the exterior normal derivative at the boundary; $c(x, t)$, for $t \in [0, T]$, $0 < T < +\infty$, $x \in \Omega$, is the compositional field (fraction of the soluto with respect to the mixture); $\theta_i(x, t)$, for $i = 1, \dots, p$, are the crystallographic orientations fields; D, κ_c, L_i, κ_i are positive constants related to the material properties. The function $\mathcal{F} = \mathcal{F}(c, \theta_1, \dots, \theta_p)$ is the local free energy density whose exact form will be presented in the next section.

In this paper we obtain a unique $(p+2)$-tuple which is a weak solution to Problem (3.1).

Throughout this paper, standard notation will be used for the required functional spaces and we denote by $\overline{f}$ the mean value of f in Ω of a given $f \in L^1(\Omega)$.

3.2 Technical hypotheses and existence of solutions

Similarly as in Fan et al. (1998), it is assumed that the local free energy $\mathcal{F}$ has the following form:

$$\begin{aligned}\mathcal{F}(c, \theta_1, \dots, \theta_p) &= -\frac{A}{2}(c - c_m)^2 + \frac{B}{4}(c - c_m)^4 + \frac{D_\alpha}{4}(c - c_\alpha)^4 \\ &+ \frac{D_\beta}{4}(c - c_\beta)^4 - \gamma \sum_{i=1}^{p} g(c, \theta_i) + \frac{\delta}{4}\sum_{i=1}^{p} \theta_i^4 + \sum_{i=1}^{p} \sum_{i \neq j = 1}^{p} \varepsilon_{ij} f(\theta_i, \theta_j).\end{aligned} \tag{3.2}$$

A, B, D_α, D_β, γ, δ , ε_{ij}, $i \neq j = 1, \dots, p$ are positive constants related to the material properties, c_α and c_β are the solubilities or equilibrium concentrations for the matrix phase and second phase, respectively, and $c_m = (c_\alpha + c_\beta)/2$.

Functions f and g are assumed to satisfy the following properties:

$$f \in C^1(\mathbf{R}^2, \mathbf{R}) \qquad \text{and} \qquad g \in C^2(\mathbf{R}^2, \mathbf{R}),$$

$$\begin{aligned}&|f(a, b) - f(u, v) + \nabla f(u, v) \cdot (u - a, v - b)| \\ &\qquad \leq F_1(u - a)^2 + F_2(v - b)^2 \ (\leq \max\{F_1, F_2\}|(u, v) - (a, b)|^2)\end{aligned} \tag{3.3}$$

and

$$|g(a, b) - g(u, v) + \nabla g(u, v) \cdot (u - a, v - b)| \leq G_1(u - a)^2 + G_2(v - b)^2 \tag{3.4}$$

for all $(u, v), (a, b) \in \mathbb{R}^2$ and fixed constants $F_1, F_2, G_1, G_2 \geq 0$. We remark that the previous assumptions on the functions f and g imply that the difference between $f(a, b)$ and $g(a, b)$ and their Taylor polynomials of degree one at (u, v), respectively, are bounded up to a multiplicative fixed constant by the square of the Euclidean distance between (u, v) and (a, b).

We also remark that the local free energy $\mathcal{F}$ is assumed to have form like the one stated above in order to comply to a requirement of Chen & Fan (1996) – Chen et al. (1997) that it should have $2p$ degenerate minima at the equilibrium concentration c_β to distinguish the $2p$ orientations differences of the second phase grains in space.

The results of this work apply, for instance, to a family of problems which contains a local free energy density given as in (3.2) but with

$$g(c, \theta_i) = g_{c_\beta}(c - c_\alpha) g_2(\theta_i) \qquad \text{and} \qquad f(\theta_i, \theta_j) = g_2(\theta_i) g_2(\theta_j)$$

where the functions g_M, $M = 2$ or c_β, are given by

$$g_M(u) = u^2 \quad \text{for } |u| \leq M \quad \text{and} \quad g_M(u) = 6M^2 - \frac{8M^3}{|u|} + \frac{3M^4}{|u|^2} \quad \text{for } |u| \geq M.$$

This example coincides in a ball of radius $\min\{c_\beta, 2\}$ with the local free energy density presented by Fan et al. (1998), having therefore the same local minima and satisfying the cited requirement.

Under the previous hypotheses we will prove the following:

THEOREM 3.1 Let $T > 0$ and $\Omega \subset R^d$, $1 \leq d \leq 3$ be a bounded domain with Lipschitz boundary. For all $c_0, \theta_{i0}, i = 1, \dots, p$, satisfying $c_0,\ \theta_{i0} \in H^1(\Omega)$, there exists a unique $(p+1)$-tuple $(c, \theta_1, \dots, \theta_p)$ such that, for $i = 1, \dots, p$,
(a) $c \in L^\infty(0, T, H^1(\Omega)) \cap L^2(0, T, H^3(\Omega))$;
(b) $\theta_i \in L^\infty(0, T, H^1(\Omega)) \cap L^2(0, T, H^2(\Omega))$;
(c) $\partial_t c \in L^2(0, T, [H^1(\Omega)]')$; $\partial_t \theta_i \in L^2(\Omega_T)$;
(d) $\partial_c \mathcal{F}(c, \theta_1, \dots, \theta_p)$, $\partial_{\theta_i} \mathcal{F}(c, \theta_1, \dots, \theta_p) \in L^2(\Omega_T)$;
(e) $c(x, 0) = c_0(x)$, $\theta_i(x, 0) = \theta_{i0}(x)$;
(f) $\partial_{\mathbf{n}} c_{|S_T} = \partial_{\mathbf{n}} \theta_{i|S_T} = 0$ in $L^2(S_T)$;
(g) $(c, \theta_1, \dots, \theta_p)$ satisfies

$$\int_0^T \langle \partial_t c, \phi \rangle dt = -\iint_{\Omega_T} D\nabla(\partial_c \mathcal{F}(c, \theta_1, \dots, \theta_p) - \kappa_c \Delta c) \nabla\phi, \tag{3.5}$$

$\forall \phi \in L^2(0, T, H^1(\Omega))$ and

$$\iint_{\Omega_T} \partial_t \theta_i \psi_i = -\iint_{\Omega_T} L_i(\partial_{\theta_i}\mathcal{F}(c, \theta_1, \dots, \theta_p) - \kappa_i \Delta\theta_i)\psi_i, \tag{3.6}$$

$\forall \psi_i \in L^2(\Omega_T), i = 1, \dots, p$, and where $\mathcal{F}$ is given by (3.2), $\langle\cdot,\cdot\rangle$ denotes the duality pairing between $H^1(\Omega)$ and its dual and $(\cdot,\cdot)$ denotes the inner product in $L^2(\Omega)$.

The above uniqueness is proved below.

LEMMA 3.1 Under the hypotheses stated in Theorem 3.1, in the $(p+1)$-tuple which solves (3.5)–(3.6) is uniquely determined.

Proof. We argue as Elliott & Luckhaus (1991). We introduce the Green's operator G: given $f \in [H^1(\Omega)]'_{null} = \{f \in [H^1(\Omega)]', \ \langle f, 1\rangle = 0\}$, we define $Gf \in H^1(\Omega)$ as the unique solution of

$$\int_\Omega \nabla Gf \nabla\psi = \langle f, \psi\rangle, \quad \forall \psi \in H^1(\Omega) \qquad \text{and} \qquad \int_\Omega Gf = 0.$$

Let $z^c = c_1 - c_2$ and $z^{\theta_i} = \theta_{i1} - \theta_{i2}$, $i = 1, \dots, p$ be the differences of two pair of solutions to (3.5)–(3.6) as in Theorem 3.1. Let

$$z^w = D[\partial_c\mathcal{F}(c_1, \theta_{11}, \dots, \theta_{p1}) - \partial_c\mathcal{F}(c_2, \theta_{12}, \dots, \theta_{p2}) - \kappa_c\Delta z^c].$$

Since equation (3.5) implies that the mean value of the composition field in Ω is conserved, we have that $(z^c, 1) = 0$ and we find from (3.5) that

$$-Gz^c_t = \overline{z^w}.$$

The definition of the Green operator and the fact that $(z^c, 1) = 0$ give

$$-(\nabla Gz^c_t, \nabla Gz^c) = -(Gz^c_t, z^c) = (\overline{z^w}, z^c) = (z^w, z^c).$$

Thus

$$\frac{1}{2}\frac{d}{dt}|\nabla Gz^c|^2 + (D[\partial_c\mathcal{F}(c_1, \theta_{11}, \dots, \theta_{p1}) - \partial_c\mathcal{F}(c_2, \theta_{12}, \dots, \theta_{p2}) - \kappa_c\Delta z^c], z^c) = 0.$$

We find from (3.6) that

$$\frac{D}{2L_i}\frac{d}{dt}|z^{\theta_i}|^2 + D\kappa_i|\nabla z^{\theta_i}|^2 + D\big(\partial_{\theta_i}\mathcal{F}(c_1, \theta_{11}, \dots, \theta_{p1}) - \partial_{\theta_i}\mathcal{F}(c_2, \theta_{12}, \dots, \theta_{p2}), z^{\theta_i}\big) = 0.$$

By adding the above equations, using the convexity of the function $[\mathcal{F}+H](c,\theta_1,\ldots,\theta_p)$ with

$$H(c,\theta_1,\ldots,\theta_p)=\frac{A}{2}(c-c_m)^2+\gamma\sum_{i=1}^{p}g(c,\theta_i)-\sum_{i=1}^{p}\sum_{i\neq j=1}^{p}\varepsilon_{ij}f(\theta_i,\theta_j),$$

and integrating by parts, we obtain

$$\begin{aligned}&\frac{1}{2}\frac{d}{dt}|\nabla\mathcal{G}z^c|^2+\kappa_c D|\nabla z^c|^2+\sum_{i=1}^{p}\left[\frac{D}{2L_i}\frac{d}{dt}|z^{\theta_i}|^2+D\kappa_i|\nabla z^{\theta_i}|^2\right]\\&\leq\big(\nabla(H(c_1,\theta_{11},\ldots,\theta_{p1})-H(c_2,\theta_{12},\ldots,\theta_{p2}))\cdot(z^c,z^{\theta_1},\ldots,z^{\theta_p}),1\big)\end{aligned}\tag{3.7}$$

In order to estimate the term at the right hand side of the above inequality, we observe that (3.3) and (3.4) imply that

$$\varepsilon_{ij}(\nabla(f(\theta_{i1},\theta_{j1})-f(\theta_{i2},\theta_{j2}))\cdot(z^{\theta_i},z^{\theta_j}),1)\leq 2\varepsilon_{ij}F_1|z^{\theta_i}|^2+2\varepsilon_{ij}F_2|z^{\theta_j}|^2$$

and

$$\gamma(\nabla(g(c_1,\theta_{i1})-g(c_2,\theta_{i2}))\cdot(z^c,z^{\theta_i}),1)\leq 2\gamma G_1|z^c|^2+2\gamma G_2|z^{\theta_i}|^2.$$

The above inequalities together (3.7) imply that

$$\begin{aligned}&\frac{1}{2}\frac{d}{dt}|\nabla\mathcal{G}z^c|^2+\frac{\kappa_c D}{2}|\nabla z^c|^2+\sum_{i=1}^{p}\left[\frac{D}{2L_i}\frac{d}{dt}|z^{\theta_i}|^2+\frac{D\kappa_i}{2}|\nabla z^{\theta_i}|^2\right]\\&\leq C\left[\|z^c\|^2_{L^2(\Omega)}+\sum_{i=1}^{p}\|z^{\theta_i}\|^2_{L^2(\Omega)}\right].\end{aligned}$$

From the definition of the Green operator, we have that $|z^c|^2=(\nabla\mathcal{G}z^c,\nabla z^c)$. Using the Hölder inequality, we can rewrite the above inequality as

$$\begin{aligned}&\frac{1}{2}\frac{d}{dt}|\nabla\mathcal{G}z^c|^2+\frac{\kappa_c D}{4}|\nabla z^c|^2+\sum_{i=1}^{p}\left[\frac{D}{2L_i}\frac{d}{dt}|z^{\theta_i}|^2+\frac{D\kappa_i}{2}|\nabla z^{\theta_i}|^2\right]\\&\leq C\left[\|\nabla\mathcal{G}z^c\|^2_{L^2(\Omega)}+\sum_{i=1}^{p}\|z^{\theta_i}\|^2_{L^2(\Omega)}\right].\end{aligned}$$

A standard Gronwall argument then yields

$$\nabla\mathcal{G}z^c=0\qquad\text{and}\qquad z^{\theta_i}=0,\quad i=1,\ldots,p,$$

since

$$\mathcal{G}z^c(0) = 0 \qquad \text{and} \qquad z^{\theta_i}(0) = 0, \quad i = 1, \dots, p.$$

The uniqueness is proved since $|z^c|^2 = (\nabla \mathcal{G} z^c, \nabla z^c) = 0$. ■

We remark that equation (3.5) implies that the average of c is conserved.

To obtain the result in Theorem 3.1, we approximate system (3.1) by a family of suitable systems and then pass to the limit. In Section 3.3, we use the results of Dal Passo, Giacomelli & Novick-Cohen (1999) to prove existence of solutions of such perturbed systems and to take the limit in these systems in the last sections.

For sake of simplicity of exposition, without loosing generality, we develop the proof for the case of dimension one and for only one orientation field variable, that is, when Ω is a bounded open interval and p is equal to one, and thus we have just one orientation field that we denote θ. In this case, the local free energy density is reduced to

$$\mathcal{F}(c, \theta) = -\frac{A}{2}(c - c_m)^2 + \frac{B}{4}(c - c_m)^4 + \frac{D_\alpha}{4}(c - c_\alpha)^4 + \frac{D_\beta}{4}(c - c_\beta)^4 - \gamma g(c, \theta) + \frac{\delta}{4}\theta^4. \tag{3.8}$$

The presented results are straightforward extended to any number of such variables.

3.3 Perturbed Systems

In this section we construct a family of perturbed systems. Such family depends on an auxiliary parameter M which controls a truncation of the local free energy $\mathcal{F}$ which will permit the application of an existence result of Dal Passo et al. (1999). We consider

$$\mathcal{F}_M(c, \theta) = \mathcal{F}(c, \theta), \quad -M \le c, \theta \le M.$$

Outside the set $[-M, M] \times [-M, M]$, we extend the above function to satisfy

$$\|\partial_c \mathcal{F}_M\|_{C^1(\mathbf{R}^2, \mathbf{R})} \le U_0(M) \qquad \text{and} \qquad \|\partial_\theta \mathcal{F}_M\|_{C(\mathbf{R}^2, \mathbf{R})} \le V_0(M), \tag{3.9}$$

$$\begin{aligned} |\partial_c \mathcal{F}_M|^2 \le K[c^6 + \theta^6 + 1] \qquad &\text{and} \qquad |\partial_{cc} \mathcal{F}_M|^2 \le K[c^4 + \theta^4 + 1], \\ |\partial_\theta \mathcal{F}_M|^2 \le K[c^6 + \theta^6 + 1] \qquad &\text{and} \qquad |\partial_{c\theta} \mathcal{F}_M|^2 \le K[c^4 + \theta^4 + 1], \end{aligned} \tag{3.10}$$

$$|\mathcal{F}_M| \le K[c^4 + \theta^4 + 1] \qquad \text{and} \qquad \mathcal{F}_M \ge m_{\mathcal{F}}, \tag{3.11}$$

$\forall M > 0$, $\forall c, \theta \in \mathbf{R}$, where $K > 0$ and $m_{\mathcal{F}}$ are constants and, for each M, $U_0(M)$ and $V_0(M)$ are also constants.

REMARK. The above properties are not restrictive since they were already satisfied by the original energy density (3.8).

The perturbed systems are given by

$$\begin{cases} \partial_t c = D\left(\partial_c \mathcal{F}_M(c,\theta) - \kappa_c c_{xx}\right)_{xx}, & (x,t) \in \Omega_T \\ \partial_t \theta = -L\left[\partial_\theta \mathcal{F}_M(c,\theta) - \kappa\theta_{xx}\right], & (x,t) \in \Omega_T \\ \partial_{\mathbf{n}} c = \partial_{\mathbf{n}}(\partial_c \mathcal{F}_M(c,\theta) - \kappa_c c_{xx}) = \partial_{\mathbf{n}}\theta = 0 & (x,t) \in S_T \\ c(x,0) = c_0(x), \quad \theta(x,0) = \theta_0(x), & x \in \Omega \end{cases} \tag{3.12}$$

To solve the above problem, we shall use the next proposition which is an existence result stated by Dal Passo et al. (1999) to the following system:

$$\begin{cases} \partial_t u = \left[q_1(u,v)\left(f_1(u,v) - \kappa_1 u_{xx}\right)_x\right]_x, & (x,t) \in \Omega_T \\ \partial_t v = -q_2(u,v)\left[f_2(u,v) - \kappa_2 v_{xx}\right], & (x,t) \in \Omega_T \\ \partial_{\mathbf{n}} u = \partial_{\mathbf{n}} u_{xx} = \partial_{\mathbf{n}} v = 0 & (x,t) \in S_T \\ u(x,0) = u_0(x), \quad v(x,0) = v_0(x), & x \in \Omega \end{cases} \tag{3.13}$$

where q_i and f_i satisfy:
(H1) $q_i \in C(\mathbf{R}^2, \mathbf{R}^+)$, with $q_{\min} \leq q_i \leq q_{\max}$ for some $0 < q_{\min} \leq q_{\max}$;
(H2) $f_1 \in C^1(\mathbf{R}^2, \mathbf{R})$ and $f_2 \in C(\mathbf{R}^2, \mathbf{R})$, with $\|f_1\|_{C^1} + \|f_2\|_{C^0} \leq F_0$ for some $F_0 > 0$.

PROPOSITION 3.1 Assuming (H1), (H2) and u_0, $v_0 \in H^1(\Omega)$, there exists a pair of functions (u, v) such that:

(i). $u \in L^\infty(0,T,H^1(\Omega)) \cap L^2(0,T,H^3(\Omega)) \cap C([0,T];H^\lambda(\Omega))$, $\lambda < 1$

(ii). $v \in L^\infty(0,T,H^1(\Omega)) \cap L^2(0,T,H^2(\Omega)) \cap C([0,T];H^\lambda(\Omega))$, $\lambda < 1$

(iii). $\partial_t u \in L^2(0,T,[H^1(\Omega)]')$, $\quad \partial_t v \in L^2(\Omega_T)$

(iv). $u(0) = u_0$ and $v(0) = v_0$ in $L^2(\Omega)$

(v). $\partial_{\mathbf{n}} u_{|S_T} = \partial_{\mathbf{n}} v_{|S_T} = 0$ in $L^2(S_T)$

(vi). (u,v) solves (3.13) in the following sense:

$$\int_0^t \langle \partial_t u, \phi \rangle = -\iint_{\Omega_t} q_1(u,v)(f_1(u,v) - \kappa_1 u_{xx})_x \phi_x, \quad \forall \phi \in L^2(0,T,H^1(\Omega))$$
$$\iint_{\Omega_t} \partial_t v \psi = -\iint_{\Omega_t} q_2(u,v)(f_2(u,v) - \kappa_2 v_{xx})\psi, \quad \forall \psi \in L^2(\Omega_T).$$

REMARK. The regularity of the test functions with respect to t allow us to obtain the integrals over $(0,t)$, instead of $(0,T)$ as originally presented by Dal Passo et al. (1999).

Since (3.9) holds, applying the above proposition, for each $M > 0$ there exists a solution (c_M, θ_M) of Problem (3.12) in the following sense

$$\int_0^t \langle \partial_t c_M, \phi \rangle = -\iint_{\Omega_t} D(\partial_c \mathcal{F}_M(c_M, \theta_M) - \kappa_c [c_M]_{xx})_x \phi_x, \tag{3.14}$$

for $\phi \in L^2(0,T,H^1(\Omega))$ and

$$\iint_{\Omega_t} \partial_t \theta_M \psi = -\iint_{\Omega_t} L(\partial_\theta \mathcal{F}_M(c_M, \theta_M) - \kappa[\theta_M]_{xx})\psi, \tag{3.15}$$

for $\psi \in L^2(\Omega_T)$.

Let us observe that equation for c_M in equation (3.14) implies that the mean value of c_M in Ω is given by

$$\overline{c_M(t)} = \overline{c_0} \tag{3.16}$$

3.4 Limit as $M \to \infty$

In this section we obtain some a priori estimates that allow taking the limit in the parameter M.

LEMMA 3.2 There exists a constant C_1 independent of M (sufficiently large) such that

(i). $||c_M||_{L^\infty(0,T,H^1(\Omega))} \leq C_1$

(ii). $||\theta_M||_{L^\infty(0,T,H^1(\Omega))} \leq C_1$

(iii). $||(\partial_c \mathcal{F}_M - \kappa_c (c_M)_{xx})_x||_{L^2(\Omega_T)} \leq C_1$

(iv). $\|\partial_\theta \mathcal{F}_M - \kappa(\theta_M)_{xx}\|_{L^2(\Omega_T)} \leq C_1$

(v). $\|\partial_t c_M\|_{L^2(0,T,[H^1(\Omega)]')} \leq C_1$

(vi). $\|\partial_t \theta_M\|_{L^2(\Omega_T)} \leq C_1$

(vii). $\|\mathcal{F}_M(c_M, \theta_M)\|_{L^\infty(0,T,L^1(\Omega))} \leq C_1$

Proof. To obtain items (iii), (iv) and (vii), we argue as Passo et al. Dal Passo et al. (1999) and Elliott & Garcke (1996). First, we observe that by the regularity of c_M and θ_M, we could take

$$\partial_c \mathcal{F}_M - \kappa_c(c_M)_{xx} \quad \text{and} \quad \partial_\theta \mathcal{F}_M - \kappa(\theta_M)_{xx}$$

as test functions in the equations (3.14) and (3.15), respectively, to obtain

$$\begin{aligned} &\int_0^t \langle \partial_t c_M, \partial_c \mathcal{F}_M - \kappa_c(c_M)_{xx}\rangle + \iint_{\Omega_t} \partial_t \theta_M \partial_\theta \mathcal{F}_M - \kappa(\theta_M)_{xx} \\ &= -\iint_{\Omega_t} D[(\partial_c \mathcal{F}_M - \kappa_c(c_M)_{xx})_x]^2 - \iint_{\Omega_t} L[\partial_\theta \mathcal{F}_M - \kappa(\theta_M)_{xx}]^2. \end{aligned} \tag{3.17}$$

Also, given a small $h > 0$, we consider the functions

$$c_{Mh}(t,x) = \frac{1}{h}\int_{t-h}^t c_M(\tau, x) d\tau$$

where we set $c_M(t,x) = c_0(x)$ for $t \leq 0$. Since $\partial_t c_{Mh}(t,x) \in L^2(\Omega_T)$, we have

$$\begin{aligned} &\int_0^t \langle (c_{Mh})_t, [\partial_c \mathcal{F}_{Mh} - \kappa_c(c_{Mh})_{xx}]\rangle dt + \iint_{\Omega_t} (\theta_M)_t[\partial_\theta \mathcal{F}_{Mh} - \kappa(\theta_M)_{xx}] \\ &= \int_\Omega \left[\frac{\kappa_c}{2}|[c_{Mh}(t)]_x|^2 + \frac{\kappa}{2}|[\theta_M]_x(t)|^2 + \mathcal{F}_{Mh}(t)\right] \\ &\qquad - \int_\Omega \left[\frac{\kappa_c}{2}|[c_0]_x|^2 + \frac{\kappa}{2}|[\theta_0]_x|^2 + \mathcal{F}_M(c_0, \theta_0)\right]. \end{aligned}$$

Taking the limit as h tends to zero in the above expression and using (3.17), we obtain

$$\begin{aligned} &\iint_{\Omega_t} D[(\partial_c \mathcal{F}_M - \kappa_c(c_M)_{xx})_x]^2 + \iint_{\Omega_t} L[\partial_\theta \mathcal{F}_M - \kappa(\theta_M)_{xx}]^2 \\ &\qquad + \frac{\kappa_c}{2}\|[c_M]_x(t)\|^2_{L^2(\Omega)} + \frac{\kappa}{2}\|[\theta_M]_x(t)\|^2_{L^2(\Omega)} + \int_\Omega \mathcal{F}_M(t) \\ &= \frac{\kappa_c}{2}\|[c_0]_x\|^2_{L^2(\Omega)} + \frac{\kappa}{2}\|[\theta_0]_x\|^2_{L^2(\Omega)} + \int_\Omega \mathcal{F}_M(c_0, \theta_0) \end{aligned}$$

for almost every $t \in (0, T]$. Using the regularity of the initial conditions (see Theorem 3.1) and (3.11), we could choose M_0, depending only on the initial conditions, to obtain for all $M > M_0$

$$\begin{aligned}\iint_{\Omega_T} D[(\partial_c \mathcal{F}_M - \kappa_c (c_M)_{xx})_x]^2 + \iint_{\Omega_T} L[\partial_\theta \mathcal{F}_M - \kappa(\theta_M)_{xx}]^2 \\ + \frac{\kappa_c}{2} \|[c_M]_x(t)\|^2_{L^2(\Omega)} + \frac{\kappa}{2} \|[\theta_M]_x(t)\|^2_{L^2(\Omega)} + \int_\Omega \mathcal{F}_M(t) \le C_1\end{aligned} \tag{3.18}$$

which implies items (iii), (iv) and (vii) since we have (3.11). Using the Poincaré inequality and (3.16), item (i) is also verified.

To prove item (vi), we choose $\psi = \partial_t \theta_M$ as a test function in (3.15), which yields

$$\begin{aligned}\iint_{\Omega_T} [\partial_t \theta_M]^2 &= - \iint_{\Omega_T} L(\partial_\theta \mathcal{F}_M - \kappa(\theta_M)_{xx}) \partial_t \theta_M \\ &\le \left(\iint_{\Omega_T} L^2 (\partial_\theta \mathcal{F}_M - \kappa(\theta_M)_{xx})^2 \right)^{1/2} \left(\iint_{\Omega_T} [\partial_t \theta_M]^2 \right)^{1/2}.\end{aligned}$$

Since we have

$$\int_\Omega \theta_M^2 \le 2 \int_\Omega |\theta_0|^2 + 2t \iint_{\Omega_T} (\partial_t \theta_M)^2 d\tau \le C_2,$$

item (vi) and (3.18), then item (ii) is verified. Finally, item (v) follows since

$$\left| \int_0^T \langle \partial_t c_M, \phi \rangle \right| \le \left(\iint_{\Omega_T} D^2 [(\partial_c \mathcal{F}_M - \kappa_c (c_M)_{xx})_x]^2 \right)^{1/2} \left(\iint_{\Omega_T} (\phi_x)^2 \right)^{1/2}$$

for all $\phi \in L^2(0, T, H^1(\Omega))$.

REMARK. From (3.18), using (3.11), we obtain

$$\begin{aligned}\iint_{\Omega_T} D[(\partial_c \mathcal{F}_M - \kappa_c (c_M)_{xx})_x]^2 + \iint_{\Omega_T} L[\partial_\theta \mathcal{F}_M - \kappa(\theta_M)_{xx}]^2 \\ + \frac{\kappa_c}{2} \|[c_M(t)]_x\|^2_{L^2(\Omega)} + \frac{\kappa}{2} \|[\theta_M]_x(t)\|^2_{L^2(\Omega)} \le C_1.\end{aligned}$$

LEMMA 3.3 For M sufficiently large, there exist a constant C_3 independent of M such that (i). $\|\partial_c \mathcal{F}_M\|_{L^2(0,T,H^1(\Omega))} \leq C_3$,

(ii). $\|\partial_\theta \mathcal{F}_M\|_{L^2(\Omega_T)} \leq C_3$,

(iii). $\|[c_M]_{xx}\|_{L^2(\Omega_T)} \leq C_3$,

(iv). $\|[\theta_M]_{xx}\|_{L^2(\Omega_T)} \leq C_3$,

Proof. First, we prove items (ii) and (iv). From Lemma 3.2(iv), we have

$$\iint_{\Omega_T} (\partial_\theta \mathcal{F}_M)^2 - 2\kappa \iint_{\Omega_T} \partial_\theta \mathcal{F}_M [\theta_M]_{xx} + \kappa^2 \iint_{\Omega_T} [\theta_M]_{xx}^2 \leq C_3. \tag{3.19}$$

Using (3.10), we obtain

$$2\kappa \partial_\theta \mathcal{F}_M [\theta_M]_{xx} \leq \frac{\kappa^2}{2}[\theta_M]_{xx}^2 + C_3[c_M^6 + \theta_M^6 + 1].$$

Thus, from Lemma 3.2(ii), it follows from (3.19) that

$$\iint_{\Omega_T} (\partial_\theta \mathcal{F}_M)^2 + \frac{\kappa^2}{2} \iint_{\Omega_T} [\theta_M]_{xx}^2 \leq C_3.$$

Now, we prove item (iii). Defining, $H_M = \partial_c \mathcal{F}_M - \kappa_c [c_M]_{xx}$, since $[c_M]_{x|S_T} = 0$, we have

$$\iint_{\Omega_T} H_M = \iint_{\Omega_T} \partial_c \mathcal{F}_M,$$

and from Lemma 3.2(iii),

$$\iint_{\Omega_T} [H_M]_x^2 \leq C_1.$$

We have

$$\iint_{\Omega_T} H_M^2 = \iint_{\Omega_T} (\partial_c \mathcal{F}_M)^2 - 2 \iint_{\Omega_T} (\partial_c \mathcal{F}_M)[c_M]_{xx} + \kappa_c^2 \iint_{\Omega_T} [c_M]_{xx}^2.$$

On the other hand, we can write

$$\iint_{\Omega_T} H_M^2 = \iint_{\Omega_T} [H_M - \overline{H_M}]^2 + \iint_{\Omega_T} \overline{H_M}^2 \leq C_P \iint_{\Omega_T} [H_M]_x^2 + \iint_{\Omega_T} (\partial_c \mathcal{F}_M)^2$$

where C_P denotes the Poincaré constant. Now, item (iii) follows from (3.10) and Lemma 3.2(i) and (ii).

Finally, using again (3.10) and Lemma 3.2(i) and (ii), we obtain

$$||\partial_c \mathcal{F}_M||^2_{L^2(\Omega_T)} \leq C_3.$$

Lemma 3.2(i) and (ii) imply that $||[\partial_c \mathcal{F}_M]_x||^2_{L^2(\Omega_T)}$ is also bounded by a constant. Thus, we have proved the item (i).

We can now state the following result.

PROPOSITION 3.2 There exists a pair (c, θ) such that:

(i). $c \in L^\infty(0, T, H^1(\Omega)) \cap L^2(0, T, H^3(\Omega))$

(ii). $\theta \in L^\infty(0, T, H^1(\Omega)) \cap L^2(0, T, H^2(\Omega))$

(iii). $\partial_t c \in L^2(0, T, [H^1(\Omega)]')$, $\quad \partial_t \theta \in L^2(\Omega_T)$

(iv). $\partial_c \mathcal{F}(c, \theta)$, $\partial_\theta \mathcal{F}(c, \theta) \in L^2(\Omega_T)$

(v). $c(0) = c_0$ and $\theta(0) = \theta_0$ in $L^2(\Omega)$

(vi). $[c]_{x|_{S_T}} = [\theta]_{x|_{S_T}} = 0$ in $L^2(S_T)$

(vii). (c, θ) solves the perturbed system (3.12) in the following sense:

$$\int_0^T \langle \partial_t c, \phi \rangle = - \iint_{\Omega_T} D[\partial_c \mathcal{F}(c, \theta) - \kappa_c(c)_{xx}]_x \phi_x$$

for all $\phi \in L^2(0, T, H^1(\Omega))$, and

$$\iint_{\Omega_T} \partial_t \theta \psi = - \iint_{\Omega_T} L(\partial_\theta \mathcal{F}(c, \theta) - \kappa \theta_{xx}) \psi$$

for all $\psi \in L^2(\Omega_T)$, and $\mathcal{F}$ is given by (3.8).

Proof. First, let us observe that from Lemma 3.2(iii) and Lemma 3.3(i), the norm of $[c_M]_{xxx}$ in $L^2(\Omega_T)$ is bounded by a constant which does not depend on M. This fact, the estimates of Lemmas 3.2 and 3.3 together with a compactness argument imply that there exists a subsequence (still denoted by $\{(c_M, \theta_M)\}$) that satisfies (as M goes to infinity)

$$
\begin{array}{llll}
c_M,\ \theta_M & \text{converge weakly-* to} & c, \theta & \text{in} \quad L^\infty(0, T, H^1(\Omega)), \\
c_M, & \text{converges weakly to} & c & \text{in} \quad L^2(0, T, H^3(\Omega)), \\
\theta_M, & \text{converges weakly to} & \theta & \text{in} \quad L^2(0, T, H^2(\Omega)), \\
\partial_t c_M, & \text{converges weakly to} & \partial_t c & \text{in} \quad L^2(0, T, [H^1(\Omega)]'), \\
\partial_t \theta_M, & \text{converges weakly to} & \partial_t \theta & \text{in} \quad L^2(\Omega_T) \\
c_M,\ \theta_M & \text{converge to} & c, \theta & \text{in} \quad L^2(\Omega_T).
\end{array}
$$

By recalling Lemmas 3.2 and 3.3, items (i)–(iii) now follow. Now, items (i) and (ii) of Lemma 3.3 imply that

$$
\begin{array}{llll}
\partial_c \mathcal{F}_M(c_M, \theta_M) & \text{converges weakly to} & \mathcal{G} & \text{in} \quad L^2(\Omega_T), \\
\partial_\theta \mathcal{F}_M(c_M, \theta_M) & \text{converges weakly to} & \mathcal{H} & \text{in} \quad L^2(\Omega_T).
\end{array}
$$

Since the strong convergence of the sequence (c_M) implies that (at least for a subsequence) $\partial_c \mathcal{F}_M(c_M, \theta_M)$ converges pointwise in Ω_T, it follows from Lemma 1.3 from Lions (1969), p. 12, that $\mathcal{G} = \partial_c \mathcal{F}(c, \theta)$. Similarly, we have $\mathcal{H} = \partial_\theta \mathcal{F}(c, \theta)$. Thus item (iv) is proved.

Item (v) is straightforward. Now, by compactness we have that

$$
\begin{array}{llll}
c_M & \text{converges to} & c & \text{in} \quad L^2(0, T, H^{2-\rho}(\Omega)), \quad \rho > 0, \\
\theta_M & \text{converges to} & \theta & \text{in} \quad L^2(0, T, H^{2-\rho}(\Omega)), \quad \rho > 0,
\end{array}
$$

which imply item (vi).

To prove item (vii), by using the previous convergences, we pass to the limit as M goes to infinity in the equations (3.14) and (3.15). Now, we complete the proof of Theorem 3.1. We argue that slight changes in the arguments previously presented prove the Theorem for higher spatial dimensions and $p > 1$.

Proof. Firstly, we discuss the case when the spatial dimension satisfies $d = 2, 3$. We start by remarking that, as observed by Dal Passo et al. (1999), Proposition 3.1 is valid for any dimension. Also, all of our previous arguments hold for dimensions $d = 2, 3$. In higher dimensions, we use an argument of elliptic regularity of the Laplacian to obtain estimates in $L^2(0, T, H^2(\Omega))$ and in $L^2(0, T, H^3(\Omega))$.

Now we explain the necessary modifications when the number of crystallographic orientations is larger than one. In this case, the local free energy density is given by

$$\begin{aligned}\mathcal{F}(c,\theta) = &-\frac{A}{2}(c-c_m)^2 + \frac{B}{4}(c-c_m)^4 + \frac{D_\alpha}{4}(c-c_\alpha)^4 + \frac{D_\beta}{4}(c-c_\beta)^4 \\ &-\gamma\sum_{i=1}^{p}\left[g(c,\theta_i) + \frac{\delta}{4}\theta_i^4 + \sum_{i\neq j=1}^{p}\varepsilon_{ij}f(\theta_i,\theta_j)\right].\end{aligned}$$

Let us note that the introduction of the mixed terms depending only on the θ_i's (the last terms) will not change greatly the arguments presented in the case when p was equal to one. In the following we point out how our previous estimates can be extended for the case when p is larger than one.

The main feature of the perturbed systems in Section 3.3 is that their corresponding local free energy density satisfy (3.9)–(3.11). Since we have (3.3), we can define a similar truncation that maintains the same properties, with such perturbed systems it is then possible to similarly establish Lemma 3.2.

As for Lemma 3.3, we treat the new terms by using the immersion of $H^1(\Omega)$ in $L^4(\Omega)$ and the estimates for the orientation field variables given in Lemma 3.2.

After we have extended the results of Lemmas 3.2 and 3.3, we can restate Proposition 3.2 without any significative change due to the introduction of the new terms.

∎

Bibliografia

Chen, L.-Q. & Fan, D. 1996 Computer simulation for a coupled grain growth and Ostwald ripening–application to Al_2O_3–Zr_2 two-phase systems. *J. Amer. Ceram. Soc.*, **79**, 1163–1168.

Chen, L.-Q. & Fan, D. 1997*a* Computer simulation of grain growth using a continuum filed model. *Acta Mater.*, **45**, 611–622.

Chen, L.-Q. & Fan, D. 1997*b* Diffusion-controlled grain growth in two-phase solids. *Acta Mater.*, **45**, 3297–3310.

Chen, L.-Q., Fan, D. & Geng, C. 1997 Computer simulation of topological evolution in 2-d grain growth using a continuum diffusion-interface filed model. *Acta Mater.*, **45**, 1115–1126.

Dal Passo, R., Giacomelli, L. & Novick-Cohen, A. 1999 Existence for an Allen-Cahn/Cahn-Hilliard system with degenerate mobility. *Interfaces and Free Boundaries*, **1**, 199–226.

Elliott, C. & Garcke, H. 1996 On the Cahn-Hilliard equation with degenerate mobility. *SIAM Journal of Mathematical Analysis*, **27**, 404–423.

Elliott, C. M. & Luckhaus, S. 1991 A generalised diffusion equation for phase separation of a multi-component mixture with interfacial free energy. Preprint **887**, IMA (Minnesota).

Fan, D., Chen, L.-Q., Chen, S. & Voorhees, P. W. 1998 Phase field formulations for modelling the Ostwald ripening in two-phase systems. *Comp. Mater. Sci.*, **9**, 329–336.

Lions, J. 1969 , *Quelques méthodes de Résolution des Problèmes aux Limites non Linéaries*, Dunod.

Capítulo 4

Redução da Ordem dos Termos Mistos

Resumo

Analisamos uma família de sistemas que acomplam uma equação do tipo Cahn-Hilliard a várias equações do tipo Allen-Cahn. Tais sistemas são análogos ao proposto por Fan, L.-Q. Chen, S. Chen e Voorhees para modelar o fenômeno "Ostwald ripening" em sistemas bifásicos. Para tal família, provamos a existência e unicidade de uma solução fraca.

A Weak Solution of a Model for Ostwald Ripening

Patrícia Nunes da Silva
nunes@ime.unicamp.br

José Luiz Boldrini
boldrini@ime.unicamp.br

Abstract

We analyze a family of systems consisting of a Cahn-Hilliard and several Allen-Cahn type equations. These systems are analogous to one proposed by Fan, L.-Q. Chen, S. Chen and Voorhees for modeling Ostwald ripening in two-phase systems. For such systems, we prove the existence and uniqueness of a weak solution.

4.1 Introduction

Ostwald ripening is a phenomenon observed in a wide variety of two-phase systems in which there is coarsening of one phase dispersed in the matrix of another. Because its practical importance, this process has been extensively studied in several degrees of generality. In particular for Ostwald ripening of anisotropic crystals, Fan et al. [4] presented a model taking in consideration both the evolution of the compositional field and of the crystallographic orientations.

Our objective in this paper is to do a mathematical analysis for a family of models of Ostwald ripening related to that presented by Fan et al. [4]. Such family is constituted of the following Cahn-Hilliard and Allen-Cahn equations:

$$\begin{cases} \partial_t c = \nabla \cdot \left[D\nabla \left(\partial_c \mathcal{F}_\lambda - \kappa_c \Delta c \right) \right], & (x,t) \in \Omega_T \\ \partial_t \theta_i = -L_i \left(\partial_{\theta_i} \mathcal{F}_\lambda - \kappa_i \Delta \theta_i \right), & (x,t) \in \Omega_T \\ \partial_{\mathbf{n}} c = \partial_{\mathbf{n}} \left(\partial_c \mathcal{F}_\lambda - \kappa_c \Delta c \right) = \partial_{\mathbf{n}} \theta_i = 0, & (x,t) \in S_T \\ c(x,0) = c_0(x), \quad \theta_i(x,0) = \theta_{i0}(x), & x \in \Omega \end{cases} \tag{4.1}$$

for $i = 1, \ldots, p$.

Here, Ω is the physical region where the Ostwald process is occurring; $\Omega_T = \Omega \times (0,T)$; $S_T = \partial\Omega \times (0,T)$; $0 < T < +\infty$; $\mathbf{n}$ denotes the unitary exterior normal vector and $\partial_{\mathbf{n}}$

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is the exterior normal derivative at the boundary; $c(x,t)$, for $t \in [0,T]$, $0 < T < +\infty$, $x \in \Omega$, is the compositional field (fraction of the soluto with respect to the mixture); $\theta_i(x,t)$, for $i = 1,\dots,p$, are the crystallographic orientations fields; D, κ_c, L_i, κ_i are positive constants related to the material properties. The function $\mathcal{F}_\lambda = \mathcal{F}_\lambda(c,\theta_1,\dots,\theta_p)$ is the local free energy density which is given by

$$\begin{aligned}\mathcal{F}_\lambda(c,\theta_1,\dots,\theta_p) &= -\frac{A}{2}(c-c_m)^2 + \frac{B}{4}(c-c_m)^4 + \frac{D_\alpha}{4}(c-c_\alpha)^4 \\ &+\frac{D_\beta}{4}(c-c_\beta)^4 + \sum_{i=1}^{p}\left[-\frac{\gamma}{2}(c-c_\alpha)^2|\theta_i|^{2-\lambda} + \frac{\delta}{4}\theta_i^4\right] + \sum_{i=1}^{p}\sum_{i\neq j=1}^{p}\frac{\varepsilon_{ij}}{2}\theta_i^2\theta_j^2\end{aligned} \tag{4.2}$$

where $\lambda \in (0,1)$; c_α and c_β are the solubilities in the matrix phase and the second phase respectively, and $c_m = (c_\alpha + c_\beta)/2$. The positive coefficients A, B, D_α, D_β, γ, δ and ε_{ij} are phenomenological parameters.

In this paper we obtain a unique $(p+1)$-tuple which is a weak solution to Problem (4.1).

Our approach to the problem is to analyze a family of suitable systems which approximate the λ-model presented at (4.1). In this analysis, we show that the approximate solutions converge to a solution of the original λ-model and this, in particular, will furnish a rigorous proof of the existence of weak solutions (see the statement of Theorem 4.1). Our approach uses an existence result presented by Passo et al. [1] for an Cahn-Hilliard/Allen-Cahn system with degenerate mobility.

Throughout this paper, standard notation will be used for the required functional spaces. We denote by $\overline{f}$ the mean value of f in Ω of a given $f \in L^1(\Omega)$.

4.2 Existence of Solutions

In this section we present our main result:

THEOREM 4.1 Let $T > 0$ and $\Omega \subset R^d$, $1 \leq d \leq 3$ be a bounded domain with Lipschitz boundary. For all c_0, θ_{i0}, $i = 1,\dots,p$, satisfying c_0, $\theta_{i0} \in H^1(\Omega)$, there exists a unique $(p+1)$-tuple $(c,\theta_1,\dots,\theta_p)$ such that, for $i = 1,\dots,p$,
(a) $c \in L^\infty(0,T,H^1(\Omega)) \cap L^2(0,T,H^3(\Omega))$;
(b) $\theta_i \in L^\infty(0,T,H^1(\Omega)) \cap L^2(0,T,H^2(\Omega))$;

(c) $\partial_t c \in L^2(0, T, [H^1(\Omega)]')$, $\partial_t \theta_i \in L^2(\Omega_T)$;
(d) $\partial_c \mathcal{F}_\lambda(c, \theta_1, \dots, \theta_p)$, $\partial_{\theta_i} \mathcal{F}_\lambda(c, \theta_1, \dots, \theta_p) \in L^2(\Omega_T)$;
(e) $c(x, 0) = c_0(x)$, $\theta_i(x, 0) = \theta_{i0}(x)$;
(f) $\partial_{\mathbf{n}} c_{|S_T} = \partial_{\mathbf{n}} \theta_{i|S_T} = 0$ in $L^2(S_T)$;
(g) $(c, \theta_1, \dots, \theta_p)$ satisfies

$$\int_0^T \langle \partial_t c, \phi \rangle dt = -\iint_{\Omega_T} D\nabla(\partial_c \mathcal{F}_\lambda(c, \theta_1, \dots, \theta_p) - \kappa_c \Delta c)\nabla\phi, \tag{4.3}$$

$\forall \phi \in L^2(0, T, H^1(\Omega))$ and

$$\iint_{\Omega_T} \partial_t \theta_i \psi_i = -\iint_{\Omega_T} L_i(\partial_{\theta_i} \mathcal{F}_\lambda(c, \theta_1, \dots, \theta_p) - \kappa_i \Delta \theta_i)\psi_i, \tag{4.4}$$

$\forall \psi_i \in L^2(\Omega_T), i = 1, \dots, p$, and where $\mathcal{F}_\lambda$ is given by (4.2), $\langle \cdot, \cdot \rangle$ denotes the duality pairing between $H^1(\Omega)$ and its dual and $(\cdot, \cdot)$ denotes the inner product in $L^2(\Omega)$.

The above uniqueness is proved below.

LEMMA 4.1 Under the hypotheses stated in Theorem 4.1, in the $(p+1)$-tuple which solves (4.3)–(4.4) are uniquely determined.

Proof. We argue as Elliott and Luckhaus [3]. We introduce the Green's operator G: given $f \in [H^1(\Omega)]'_{null} = \{f \in [H^1(\Omega)]', \langle f, 1 \rangle = 0\}$, we define $Gf \in H^1(\Omega)$ as the unique solution of

$$\int_\Omega \nabla Gf \nabla \psi = \langle f, \psi \rangle, \quad \forall \psi \in H^1(\Omega) \qquad \text{and} \qquad \int_\Omega Gf = 0.$$

Let $z^c = c_1 - c_2$ and $z^{\theta_i} = \theta_{i1} - \theta_{i2}$, $i = 1, \dots, p$, be the differences of two pair of solutions to (4.3)–(4.4) as in Theorem 4.1. Let

$$z^w = D[\partial_c \mathcal{F}_\lambda(c_1, \theta_{11}, \dots, \theta_{p1}) - \partial_c \mathcal{F}_\lambda(c_2, \theta_{12}, \dots, \theta_{p2}) - \kappa_c \Delta z^c].$$

Since equation (4.3) implies that the mean value of the composition field in Ω is conserved, we have that $(z^c, 1) = 0$ and we find from (4.3) that

$$-Gz^c_t = \overline{z^w}.$$

The definition of the Green operator and the fact that $(z^c, 1) = 0$ give

$$-(\nabla G z_t^c, \nabla G z^c) = -(G z_t^c, z^c) = (\overline{z^w}, z^c) = (z^w, z^c).$$

Thus

$$\frac{1}{2}\frac{d}{dt}|\nabla G z^c|^2 + (D[\partial_c \mathcal{F}_\lambda(c_1, \theta_{11}, \dots, \theta_{p1}) - \partial_c \mathcal{F}_\lambda(c_2, \theta_{12}, \dots, \theta_{p2}) - \kappa_c \Delta z^c], z^c) = 0.$$

We find from (4.4) that

$$\frac{D}{2L_i}\frac{d}{dt}|z^{\theta_i}|^2 + D\kappa_i|\nabla z^{\theta_i}|^2 + D\big(\partial_{\theta_i}\mathcal{F}_\lambda(c_1, \theta_{11}, \dots, \theta_{p1}) - \partial_{\theta_i}\mathcal{F}_\lambda(c_2, \theta_{12}, \dots, \theta_{p2}), z^{\theta_i}\big) = 0.$$

By adding the above equations, using the convexity of the function $[\mathcal{F}_\lambda + H_\lambda](c, \theta_1, \dots, \theta_p)$ with

$$H_\lambda(c, \theta_1, \dots, \theta_p) = \frac{A}{2}(c - c_m)^2 + \frac{\gamma}{2}\sum_{i=1}^{p}(c - c_\alpha)^2|\theta_i|^{2-\lambda} - \sum_{i=1}^{p}\sum_{i \neq j = 1}^{p}\frac{\varepsilon_{ij}}{2}\theta_i^2\theta_j^2,$$

and integrating by parts, we obtain

$$\begin{aligned}&\frac{1}{2}\frac{d}{dt}|\nabla \mathcal{G} z^c|^2 + \kappa_c D|\nabla z^c|^2 + \sum_{i=1}^{p}\left[\frac{D}{2L_i}\frac{d}{dt}|z^{\theta_i}|^2 + D\kappa_i|\nabla z^{\theta_i}|^2\right] \\ &\leq \big(\nabla(H_\lambda(c_1, \theta_{11}, \dots, \theta_{p1}) - H_\lambda(c_2, \theta_{12}, \dots, \theta_{p2})) \cdot (z^c, z^{\theta_1}, \dots, z^{\theta_p}), 1\big)\end{aligned} \tag{4.5}$$

In order to estimate the term at the right hand side of the above inequality, we observe that since $c_i, \theta_{ij} \in L^\infty(0, T, H^1(\Omega))$, we have

$$\begin{aligned}\gamma((c_1 - c_\alpha)|\theta_{i1}|^{2-\lambda} - (c_2 - c_\alpha)|\theta_{i2}|^{2-\lambda}, z^c) &= \gamma(z^c|\theta_{i1}|^{2-\lambda} + (c_2 - c_\alpha)(|\theta_{i1}|^{2-\lambda} - |\theta_{i2}|^{2-\lambda}), z^c) \\ &\leq \frac{\kappa_c D}{4p}\|\nabla z^c\|^2_{L^2(\Omega)} + \frac{D\kappa_i}{8p}\|\nabla z^{\theta_i}\|^2_{L^2(\Omega)} + C\|z^{\theta_i}\|^2_{L^2(\Omega)} + C\|z^c\|^2_{L^2(\Omega)},\end{aligned}$$

$$\begin{aligned}&\frac{(2-\lambda)\gamma}{2}((c_1 - c_\alpha)^2|\theta_{i1}|^{1-\lambda}\operatorname{sgn}(\theta_{i1}) - (c_2 - c_\alpha)^2|\theta_{i2}|^{1-\lambda}\operatorname{sgn}(\theta_{i2}), z^{\theta_i}) \\ &\qquad \leq \frac{\kappa_c D}{4p}\|\nabla z^c\|^2_{L^2(\Omega)} + \frac{D\kappa_i}{8p}\|\nabla z^{\theta_i}\|^2_{L^2(\Omega)} + C\|z^{\theta_i}\|^2_{L^2(\Omega)} + C\|z^c\|^2_{L^2(\Omega)}\end{aligned}$$

and

$$\varepsilon_{ij}(\theta_{i1}\theta_{j1}^2 - \theta_{i2}\theta_{j2}^2, z^{\theta_i}) = \varepsilon_{ij}(z^{\theta_i}\theta_{j1}^2 + \theta_{i2}(\theta_{j1}+\theta_{j2})(\theta_{j1}-\theta_{j2}), z^{\theta_i})$$
$$\leq \frac{D\kappa_i}{8(p-1)}\|\nabla z^{\theta_i}\|^2_{L^2(\Omega)} + \frac{D\kappa_j}{8(p-1)}\|\nabla z^{\theta_j}\|^2_{L^2(\Omega)} + C\|z^{\theta_i}\|^2_{L^2(\Omega)} + C\|z^{\theta_j}\|^2_{L^2(\Omega)}.$$

The above inequalities together (4.5) imply that

$$\frac{1}{2}\frac{d}{dt}|\nabla\mathcal{G}z^c|^2 + \frac{\kappa_c D}{2}|\nabla z^c|^2 + \sum_{i=1}^{p}\left[\frac{D}{2L_i}\frac{d}{dt}|z^{\theta_i}|^2 + \frac{D\kappa_i}{2}|\nabla z^{\theta_i}|^2\right]$$
$$\leq C\left[\|z^c\|^2_{L^2(\Omega)} + \sum_{i=1}^{p}\|z^{\theta_i}\|^2_{L^2(\Omega)}\right].$$

From the definition of the Green operator, we have that $|z^c|^2 = (\nabla\mathcal{G}z^c, \nabla z^c)$. Using the Hölder inequality, we can rewrite the above inequality as

$$\frac{1}{2}\frac{d}{dt}|\nabla\mathcal{G}z^c|^2 + \frac{\kappa_c D}{4}|\nabla z^c|^2 + \sum_{i=1}^{p}\left[\frac{D}{2L_i}\frac{d}{dt}|z^{\theta_i}|^2 + \frac{D\kappa_i}{2}|\nabla z^{\theta_i}|^2\right]$$
$$\leq C\left[\|\nabla\mathcal{G}z^c\|^2_{L^2(\Omega)} + \sum_{i=1}^{p}\|z^{\theta_i}\|^2_{L^2(\Omega)}\right].$$

A standard Gronwall argument then yields uniqueness since

$$z^c(0) = 0 \qquad \text{and} \qquad z^{\theta_i}(0) = 0, \quad i = 1, \ldots, p.$$

■

To obtain the result in Theorem 4.1, we approximate system (4.1) by a family of suitable systems and then pass to the limit. In Section 4.3, we use the results of Passo et al. [1] to prove existence of solutions of such perturbed systems and to take the limit in these systems in the last sections.

For sake of simplicity of exposition, without loosing generality, we develop the proof for the case of dimension one and for only one orientation field variable, that is, when Ω is a bounded open interval and p is equal to one, and thus we have just one orientation field that we denote θ. In this case, the local free energy density is reduced to

$$\mathcal{F}_\lambda(c,\theta) = -\frac{A}{2}(c-c_m)^2 + \frac{B}{4}(c-c_m)^4 + \frac{D_\alpha}{4}(c-c_\alpha)^4 + \frac{D_\beta}{4}(c-c_\beta)^4$$
$$-\frac{\gamma}{2}(c-c_\alpha)^2|\theta|^{2-\lambda} + \frac{\delta}{4}\theta^4. \tag{4.6}$$

Even though the crossed terms of (4.2) involving the orientation field variables are absent in above expression, when extending the result for p greater than one, they will not bring any difficulty as we point out at the end of the paper.

4.3 Perturbed Systems

In this section we construct a family of perturbed systems. Such family depends on an auxiliary parameter M which controls a truncation of the local free energy $\mathcal{F}_\lambda$ which will permit the application of an existence result of Passo et al. [1]. We consider

$$\mathcal{F}_{\lambda M}(c,\theta) = \mathcal{F}_\lambda(c,\theta), \quad -M \le c, \theta \le M.$$

Outside the set $[-M, M] \times [-M, M]$, we extend the above function to satisfy

$$\|\partial_c \mathcal{F}_{\lambda M}\|_{C^1(\mathbf{R}^2,\mathbf{R})} \le U_0(M) \qquad \text{and} \qquad \|\partial_\theta \mathcal{F}_{\lambda M}\|_{C(\mathbf{R}^2,\mathbf{R})} \le V_0(M), \tag{4.7}$$

$$\begin{aligned} |\partial_c \mathcal{F}_{\lambda M}|^2 \le K[c^6 + \theta^6 + 1] \qquad &\text{and} \qquad |\partial_{cc} \mathcal{F}_{\lambda M}|^2 \le K[c^4 + \theta^4 + 1], \\ |\partial_\theta \mathcal{F}_{\lambda M}|^2 \le K[c^6 + \theta^6 + 1] \qquad &\text{and} \qquad |\partial_{c\theta} \mathcal{F}_{\lambda M}|^2 \le K[c^4 + \theta^4 + 1], \end{aligned} \tag{4.8}$$

$$|\mathcal{F}_{\lambda M}| \le K[c^4 + \theta^4 + 1] \qquad \text{and} \qquad \mathcal{F}_{\lambda M} \ge m_{\mathcal{F}}(\lambda), \tag{4.9}$$

$\forall M > 0$, $\forall c, \theta \in \mathbf{R}$, where $K > 0$ is a constant, for each λ, $m_{\mathcal{F}}(\lambda)$ is a constant, and, for each M, $U_0(M)$ and $V_0(M)$ are also constants.

REMARK. The above properties are not restrictive since they were already satisfied by the original energy density (4.6).

The perturbed systems are given by

$$\begin{cases} \partial_t c = D\left(\partial_c \mathcal{F}_{\lambda M}(c,\theta) - \kappa_c c_{xx}\right)_{xx}, & (x,t) \in \Omega_T \\ \partial_t \theta = -L\left[\partial_\theta \mathcal{F}_{\lambda M}(c,\theta) - \kappa \theta_{xx}\right], & (x,t) \in \Omega_T \\ \partial_{\mathbf{n}} c = \partial_{\mathbf{n}}(\partial_c \mathcal{F}_{\lambda M}(c,\theta) - \kappa_c c_{xx}) = \partial_{\mathbf{n}} \theta = 0, & (x,t) \in S_T \\ c(x,0) = c_0(x), \quad \theta(x,0) = \theta_0(x), & x \in \Omega \end{cases} \tag{4.10}$$

To solve the above problem, we shall use the next proposition which is an existence result stated by Passo et al. [1] to the following system:

$$\begin{cases} \partial_t u = \left[q_1(u,v)\left(f_1(u,v) - \kappa_1 u_{xx}\right)_x\right]_x, & (x,t) \in \Omega_T \\ \partial_t v = -q_2(u,v)\left[f_2(u,v) - \kappa_2 v_{xx}\right], & (x,t) \in \Omega_T \\ \partial_{\mathbf{n}} u = \partial_{\mathbf{n}} u_{xx} = \partial_{\mathbf{n}} v = 0, & (x,t) \in S_T \\ u(x,0) = u_0(x), \quad v(x,0) = v_0(x), & x \in \Omega \end{cases} \tag{4.11}$$

where q_i and f_i satisfy:

(H1) $q_i \in C(\mathbf{R}^2, \mathbf{R}^+)$, with $q_{\min} \leq q_i \leq q_{\max}$ for some $0 < q_{\min} \leq q_{\max}$;
(H2) $f_1 \in C^1(\mathbf{R}^2, \mathbf{R})$ and $f_2 \in C(\mathbf{R}^2, \mathbf{R})$, with $\|f_1\|_{C^1} + \|f_2\|_{C^0} \leq F_0$ for some $F_0 > 0$.

PROPOSITION 4.1 Assuming (H1), (H2) and u_0, $v_0 \in H^1(\Omega)$, there exists a pair of functions (u, v) such that:

(i). $u \in L^\infty(0, T, H^1(\Omega)) \cap L^2(0, T, H^3(\Omega)) \cap C([0,T]; H^\rho(\Omega))$, $\rho < 1$

(ii). $v \in L^\infty(0, T, H^1(\Omega)) \cap L^2(0, T, H^2(\Omega)) \cap C([0,T]; H^\rho(\Omega))$, $\rho < 1$

(iii). $\partial_t u \in L^2(0, T, [H^1(\Omega)]')$, $\quad \partial_t v \in L^2(\Omega_T)$

(iv). $u(0) = u_0$ and $v(0) = v_0$ in $L^2(\Omega)$

(v). $\partial_{\mathbf{n}} u_{|S_T} = \partial_{\mathbf{n}} v_{|S_T} = 0$ in $L^2(S_T)$

(vi). (u, v) solves (4.11) in the following sense:

$$\int_0^t \langle \partial_t u, \phi \rangle = -\iint_{\Omega_t} q_1(u,v)(f_1(u,v) - \kappa_1 u_{xx})_x \phi_x, \quad \forall \phi \in L^2(0, T, H^1(\Omega))$$

$$\iint_{\Omega_t} \partial_t v \psi = -\iint_{\Omega_t} q_2(u,v)(f_2(u,v) - \kappa_2 v_{xx})\psi, \quad \forall \psi \in L^2(\Omega_T).$$

REMARK. The regularity of the test functions with respect to t allow us to obtain the integrals over $(0, t)$, instead of $(0, T)$ as originally presented by Passo et al. [1].

Since (4.7) holds, applying the above proposition, for each $M > 0$ there exists a solution $(c_{\lambda M}, \theta_{\lambda M})$ of Problem (4.10) in the following sense

$$\int_0^t \langle \partial_t c_{\lambda M}, \phi \rangle = -\iint_{\Omega_t} D(\partial_c \mathcal{F}_{\lambda M}(c_{\lambda M}, \theta_{\lambda M}) - \kappa_c [c_{\lambda M}]_{xx})_x \phi_x, \tag{4.12}$$

for $\phi \in L^2(0,T,H^1(\Omega))$ and

$$\iint_{\Omega_t} \partial_t\theta_{\lambda M}\psi = -\iint_{\Omega_t} L(\partial_\theta \mathcal{F}_{\lambda M}(c_{\lambda M},\theta_{\lambda M}) - \kappa[\theta_{\lambda M}]_{xx})\psi, \tag{4.13}$$

for $\psi \in L^2(\Omega_T)$.

Let us observe that equation for $c_{\lambda M}$ in equation (4.12) implies that the mean value of $c_{\lambda M}$ in Ω is given by

$$\overline{c_{\lambda M}(t)} = \overline{c_0} \tag{4.14}$$

4.4 Limit as $M \to \infty$

In this section we obtain some a priori estimates that allow taking the limit in the parameter M.

LEMMA 4.2 There exists a constant C_1 independent of M (sufficiently large) such that

(i). $||c_{\lambda M}||_{L^\infty(0,T,H^1(\Omega))} \leq C_1$

(ii). $||\theta_{\lambda M}||_{L^\infty(0,T,H^1(\Omega))} \leq C_1$

(iii). $||(\partial_c\mathcal{F}_{\lambda M} - \kappa_c(c_{\lambda M})_{xx})_x||_{L^2(\Omega_T)} \leq C_1$

(iv). $||\partial_\theta\mathcal{F}_{\lambda M} - \kappa(\theta_{\lambda M})_{xx}||_{L^2(\Omega_T)} \leq C_1$

(v). $||\partial_t c_{\lambda M}||_{L^2(0,T,[H^1(\Omega)]')} \leq C_1$

(vi). $||\partial_t\theta_{\lambda M}||_{L^2(\Omega_T)} \leq C_1$

(vii). $||\mathcal{F}_{\lambda M}(c_{\lambda M},\theta_{\lambda M})||_{L^\infty(0,T,L^1(\Omega))} \leq C_1$

Proof. To obtain items (iii), (iv) and (vii), we argue as Passo et al. [1] and Elliott and Garcke [2]. First, we observe that by the regularity of $c_{\lambda M}$ and $\theta_{\lambda M}$, we could take

$$\partial_c\mathcal{F}_{\lambda M} - \kappa_c(c_{\lambda M})_{xx} \quad \text{and} \quad \partial_\theta\mathcal{F}_{\lambda M} - \kappa(\theta_{\lambda M})_{xx}$$

as test functions in the equations (4.12) and (4.13), respectively, to obtain

$$\begin{aligned}\int_0^t \langle \partial_t c_{\lambda M}, \partial_c \mathcal{F}_{\lambda M} - \kappa_c (c_{\lambda M})_{xx}\rangle + \iint_{\Omega_t} \partial_t \theta_{\lambda M} \partial_\theta \mathcal{F}_{\lambda M} - \kappa(\theta_{\lambda M})_{xx} \\ = -\iint_{\Omega_t} D[(\partial_c \mathcal{F}_{\lambda M} - \kappa_c (c_{\lambda M})_{xx})_x]^2 - \iint_{\Omega_t} L[\partial_\theta \mathcal{F}_{\lambda M} - \kappa(\theta_{\lambda M})_{xx}]^2.\end{aligned} \tag{4.15}$$

Also, given a small $h > 0$, we consider the functions

$$\mathcal{F}_{\lambda Mh} = \mathcal{F}_{\lambda M}(c_{\lambda Mh}, \theta_{\lambda M}) \qquad \text{and} \qquad c_{\lambda Mh}(t,x) = \frac{1}{h}\int_{t-h}^t c_{\lambda M}(\tau, x)d\tau$$

where we set $c_{\lambda M}(t,x) = c_0(x)$ for $t \leq 0$. Since $\partial_t c_{\lambda Mh}(t,x) \in L^2(\Omega_T)$, we have

$$\begin{aligned}&\int_0^t \langle (c_{\lambda Mh})_t, [\partial_c \mathcal{F}_{\lambda Mh} - \kappa_c (c_{\lambda Mh})_{xx}]\rangle dt + \iint_{\Omega_t} (\theta_{\lambda M})_t [\partial_\theta \mathcal{F}_{\lambda Mh} - \kappa(\theta_{\lambda M})_{xx}] \\ &= \int_\Omega \left[\frac{\kappa_c}{2}|[c_{\lambda Mh}(t)]_x|^2 + \frac{\kappa}{2}|[\theta_{\lambda M}]_x(t)|^2 + \mathcal{F}_{\lambda Mh}(t)\right] - \int_\Omega \left[\frac{\kappa_c}{2}|[c_0]_x|^2 + \frac{\kappa}{2}|[\theta_0]_x|^2 + \mathcal{F}_{\lambda M}(c_0, \theta_0)\right].\end{aligned}$$

Taking the limit as h tends to zero in the above expression and using (4.15), we obtain

$$\begin{aligned}\iint_{\Omega_t} D[(\partial_c \mathcal{F}_{\lambda M} - \kappa_c (c_{\lambda M})_{xx})_x]^2 + \iint_{\Omega_t} L[\partial_\theta \mathcal{F}_{\lambda M} - \kappa(\theta_{\lambda M})_{xx}]^2 \\ + \frac{\kappa_c}{2}\|[c_{\lambda M}]_x(t)\|^2_{L^2(\Omega)} + \frac{\kappa}{2}\|[\theta_{\lambda M}]_x(t)\|^2_{L^2(\Omega)} + \int_\Omega \mathcal{F}_{\lambda M}(t) \\ = \frac{\kappa_c}{2}\|[c_0]_x\|^2_{L^2(\Omega)} + \frac{\kappa}{2}\|[\theta_0]_x\|^2_{L^2(\Omega)} + \int_\Omega \mathcal{F}_{\lambda M}(c_0, \theta_0)\end{aligned}$$

for almost every $t \in (0,T]$. Using the regularity of the initial conditions (see Theorem 4.1) and (4.9), we could choose M_0, depending only on the initial conditions, to obtain for all $M > M_0$

$$\begin{aligned}\iint_{\Omega_T} D[(\partial_c \mathcal{F}_{\lambda M} - \kappa_c (c_{\lambda M})_{xx})_x]^2 + \iint_{\Omega_T} L[\partial_\theta \mathcal{F}_{\lambda M} - \kappa(\theta_{\lambda M})_{xx}]^2 \\ + \frac{\kappa_c}{2}\|[c_{\lambda M}]_x(t)\|^2_{L^2(\Omega)} + \frac{\kappa}{2}\|[\theta_{\lambda M}]_x(t)\|^2_{L^2(\Omega)} + \int_\Omega \mathcal{F}_{\lambda M}(t) \leq C_1\end{aligned} \tag{4.16}$$

which implies items (iii), (iv) and (vii) since we have (4.9). Using the Poincaré inequality and (4.14), item (i) is also verified.

To prove item (vi), we choose $\psi = \partial_t\theta_{\lambda M}$ as a test function in (4.13), which yields

$$\iint_{\Omega_T}[\partial_t\theta_{\lambda M}]^2 = -\iint_{\Omega_T} L(\partial_\theta\mathcal{F}_{\lambda M} - \kappa(\theta_{\lambda M})_{xx})\partial_t\theta_{\lambda M}$$
$$\leq \left(\iint_{\Omega_T} L^2(\partial_\theta\mathcal{F}_{\lambda M} - \kappa(\theta_{\lambda M})_{xx})^2\right)^{1/2}\left(\iint_{\Omega_T}[\partial_t\theta_{\lambda M}]^2\right)^{1/2}.$$

Since we have

$$\int_\Omega \theta_{\lambda M}^2 \leq 2\int_\Omega |\theta_0|^2 + 2t\iint_{\Omega_T}(\partial_t\theta_{\lambda M})^2 d\tau \leq C_2,$$

item (vi) and (4.16), then item (ii) is verified. Finally, item (v) follows since

$$\left|\int_0^T\langle\partial_t c_{\lambda M},\phi\rangle\right| \leq \left(\iint_{\Omega_T} D^2[(\partial_c\mathcal{F}_{\lambda M} - \kappa_c(c_{\lambda M})_{xx})_x]^2\right)^{1/2}\left(\iint_{\Omega_T}(\phi_x)^2\right)^{1/2}$$

for all $\phi \in L^2(0,T,H^1(\Omega))$.

REMARK. From (4.16), using (4.9), we obtain

$$\iint_{\Omega_T} D[(\partial_c\mathcal{F}_{\lambda M} - \kappa_c(c_{\lambda M})_{xx})_x]^2 + \iint_{\Omega_T} L[\partial_\theta\mathcal{F}_{\lambda M} - \kappa(\theta_{\lambda M})_{xx}]^2$$
$$+\frac{\kappa_c}{2}\|[c_{\lambda M}(t)]_x\|^2_{L^2(\Omega)} + \frac{\kappa}{2}\|[\theta_{\lambda M}]_x(t)\|^2_{L^2(\Omega)} \leq C_1.$$

LEMMA 4.3 For M sufficiently large, there exist a constant C_3 independent of M such that

(i). $\|\partial_c\mathcal{F}_{\lambda M}\|_{L^2(0,T,H^1(\Omega))} \leq C_3$,

(ii). $\|\partial_\theta\mathcal{F}_{\lambda M}\|_{L^2(\Omega_T)} \leq C_3$,

(iii). $\|[c_{\lambda M}]_{xx}\|_{L^2(\Omega_T)} \leq C_3$,

(iv). $\|[\theta_{\lambda M}]_{xx}\|_{L^2(\Omega_T)} \leq C_3$,

Proof. First, we prove items (ii) and (iv). From Lemma 4.2(iv), we have

$$\iint_{\Omega_T}(\partial_\theta\mathcal{F}_{\lambda M})^2 - 2\kappa\iint_{\Omega_T}\partial_\theta\mathcal{F}_{\lambda M}[\theta_{\lambda M}]_{xx} + \kappa^2\iint_{\Omega_T}[\theta_{\lambda M}]^2_{xx} \leq C_3. \tag{4.17}$$

Using (4.8), we obtain

$$2\kappa\partial_\theta\mathcal{F}_{\lambda M}[\theta_{\lambda M}]_{xx} \leq \frac{\kappa^2}{2}[\theta_{\lambda M}]_{xx}^2 + C_3[c_{\lambda M}^6 + \theta_{\lambda M}^6 + 1].$$

Thus, from Lemma 4.2(ii), it follows from (4.17) that

$$\iint_{\Omega_T}(\partial_\theta\mathcal{F}_{\lambda M})^2 + \frac{\kappa^2}{2}\iint_{\Omega_T}[\theta_{\lambda M}]_{xx}^2 \leq C_3.$$

Now, we prove item (iii). Defining, $H_{\lambda M} = \partial_c\mathcal{F}_{\lambda M} - \kappa_c[c_{\lambda M}]_{xx}$, since $[c_{\lambda M}]_{x|S_T} = 0$, we have

$$\iint_{\Omega_T} H_{\lambda M} = \iint_{\Omega_T}\partial_c\mathcal{F}_{\lambda M},$$

and from Lemma 4.2(iii),

$$\iint_{\Omega_T}[H_{\lambda M}]_x^2 \leq C_1.$$

We have

$$\iint_{\Omega_T} H_{\lambda M}^2 = \iint_{\Omega_T}(\partial_c\mathcal{F}_{\lambda M})^2 - 2\iint_{\Omega_T}(\partial_c\mathcal{F}_{\lambda M})[c_{\lambda M}]_{xx} + \kappa_c^2\iint_{\Omega_T}[c_{\lambda M}]_{xx}^2.$$

On the other hand, we can write

$$\begin{aligned}\iint_{\Omega_T} H_{\lambda M}^2 &= \iint_{\Omega_T}[H_{\lambda M} - \overline{H_{\lambda M}}]^2 + \iint_{\Omega_T}\overline{H_{\lambda M}}^2 \\ &\leq C_P\iint_{\Omega_T}[H_{\lambda M}]_x^2 + \iint_{\Omega_T}(\partial_c\mathcal{F}_{\lambda M})^2\end{aligned}$$

where C_P denotes the Poincaré constant. Now, item (iii) follows from (4.8) and Lemma 4.2(i) and (ii).

Finally, using again (4.8) and Lemma 4.2(i) and (ii), we obtain

$$\|\partial_c\mathcal{F}_{\lambda M}\|_{L^2(\Omega_T)}^2 \leq C_3.$$

Lemma 4.2(i) and (ii) imply that $\|[\partial_c\mathcal{F}_{\lambda M}]_x\|_{L^2(\Omega_T)}^2$ is also bounded by a constant. Thus, we have proved the item (i).

We can now state the following result.

PROPOSITION 4.2 There exists a pair $(c_\lambda, \theta_\lambda)$ such that:

(i). $c_\lambda \in L^\infty(0,T,H^1(\Omega)) \cap L^2(0,T,H^3(\Omega))$

(ii). $\theta_\lambda \in L^\infty(0,T,H^1(\Omega)) \cap L^2(0,T,H^2(\Omega))$

(iii). $\partial_t c_\lambda \in L^2(0,T,[H^1(\Omega)]')$, $\quad \partial_t\theta_\lambda \in L^2(\Omega_T)$

(iv). $\partial_c\mathcal{F}_\lambda(c_\lambda,\theta_\lambda)$, $\partial_\theta\mathcal{F}_\lambda(c_\lambda,\theta_\lambda) \in L^2(\Omega_T)$

(v). $c_\lambda(0) = c_0$ and $\theta_\lambda(0) = \theta_0$ in $L^2(\Omega)$

(vi). $[c_\lambda]_{x|_{S_T}} = [\theta_\lambda]_{x|_{S_T}} = 0$ in $L^2(S_T)$

(vii). $(c_\lambda, \theta_\lambda)$ solves the perturbed system (4.10) in the following sense:

$$\int_0^T \langle \partial_t c_\lambda, \phi\rangle = -\iint_{\Omega_T} D[\partial_c\mathcal{F}_\lambda(c_\lambda,\theta_\lambda) - \kappa_c(c_\lambda)_{xx}]_x\phi_x$$

for all $\phi \in L^2(0,T,H^1(\Omega))$, and

$$\iint_{\Omega_T} \partial_t\theta_\lambda\psi = -\iint_{\Omega_T} L(\partial_\theta\mathcal{F}_\lambda(c_\lambda,\theta_\lambda) - \kappa(\theta_\lambda)_{xx})\psi$$

for all $\psi \in L^2(\Omega_T)$, and $\mathcal{F}_\lambda$ is given by (4.6).

Proof. First, let us observe that from Lemma 4.2(iii) and Lemma 4.3(i), the norm of $[c_{\lambda M}]_{xxx}$ in $L^2(\Omega_T)$ is bounded by a constant which does not depend on M. This fact, the estimates of Lemmas 4.2 and 4.3 together with a compactness argument imply that there exists a subsequence (still denoted by $\{(c_{\lambda M}, \theta_{\lambda M})\}$) that satisfies (as M goes to infinity)

$$\begin{array}{llll}
c_{\lambda M},\ \theta_{\lambda M} & \text{converge weakly-* to} & c_\lambda, \theta_\lambda & \text{in } L^\infty(0,T,H^1(\Omega)),\\
c_{\lambda M}, & \text{converges weakly to} & c_\lambda & \text{in } L^2(0,T,H^3(\Omega)),\\
\theta_{\lambda M}, & \text{converges weakly to} & \theta_\lambda & \text{in } L^2(0,T,H^2(\Omega)),\\
\partial_t c_{\lambda M}, & \text{converges weakly to} & \partial_t c_\lambda & \text{in } L^2(0,T,[H^1(\Omega)]'),\\
\partial_t\theta_{\lambda M}, & \text{converges weakly to} & \partial_t\theta_\lambda & \text{in } L^2(\Omega_T)\\
c_{\lambda M},\ \theta_{\lambda M} & \text{converge to} & c_\lambda, \theta_\lambda & \text{in } L^2(\Omega_T).
\end{array}$$

By recalling Lemmas 4.2 and 4.3, items (i)–(iii) now follow. Now, items (i) and (ii) of Lemma 4.3 imply that

$$\partial_c \mathcal{F}_{\lambda M}(c_{\lambda M}, \theta_{\lambda M}) \quad \text{converges weakly to} \quad \mathcal{G} \quad \text{in} \quad L^2(\Omega_T),$$
$$\partial_\theta \mathcal{F}_{\lambda M}(c_{\lambda M}, \theta_{\lambda M}) \quad \text{converges weakly to} \quad \mathcal{H} \quad \text{in} \quad L^2(\Omega_T).$$

Since the strong convergence of the sequence $(c_{\lambda M})$ implies that (at least for a subsequence) $\partial_c \mathcal{F}_{\lambda M}(c_{\lambda M}, \theta_{\lambda M})$ converges pointwise in Ω_T, it follows from Lemma 1.3 from Lions [5], p. 12, that $\mathcal{G} = \partial_c \mathcal{F}_\lambda(c_\lambda, \theta_\lambda)$. Similarly, we have $\mathcal{H} = \partial_\theta \mathcal{F}_\lambda(c_\lambda, \theta_\lambda)$. Thus item (iv) is proved.

Item (v) is straightforward. Now, by compactness we have that

$$c_{\lambda M} \quad \text{converges to} \quad c_\lambda \quad \text{in} \quad L^2(0, T, H^{2-\rho}(\Omega)), \quad \rho > 0,$$
$$\theta_{\lambda M} \quad \text{converges to} \quad \theta_\lambda \quad \text{in} \quad L^2(0, T, H^{2-\rho}(\Omega)), \quad \rho > 0,$$

which imply item (vi).

To prove item (vii), by using the previous convergences, we pass to the limit as M goes to infinity in the equations (4.12) and (4.13). Now, we complete the proof of Theorem 4.1. We argue that slight changes in the arguments previously presented prove the Theorem for higher spatial dimensions and $p > 1$.

Proof. Firstly, we discuss the case when the spatial dimension satisfies $d = 2, 3$. We start by remarking that, as observed by Passo et al. [1], Proposition 4.1 is valid for any dimension. Also, all of our previous arguments hold for dimensions $d = 2, 3$. In higher dimensions, we use an argument of elliptic regularity of the Laplacian to obtain estimates in $L^2(0, T, H^2(\Omega))$ and in $L^2(0, T, H^3(\Omega))$.

Now we explain the necessary modifications when the number of crystallographic orientations is larger than one. In this case, the local free energy density is given by

$$\mathcal{F}_\lambda(c, \theta) = -\frac{A}{2}(c - c_m)^2 + \frac{B}{4}(c - c_m)^4 + \frac{D_\alpha}{4}(c - c_\alpha)^4 + \frac{D_\beta}{4}(c - c_\beta)^4$$
$$-\frac{\gamma}{2}\sum_{i=1}^{p}\left[(c - c_\alpha)^2|\theta_i|^{2-\lambda} + \frac{\delta}{4}\theta_i^4 + \sum_{i \neq j = 1}^{p}\frac{\varepsilon_{ij}}{2}\theta_i^2\theta_j^2\right].$$

Let us note that increasing the introduction of the mixed terms depending only on the θ_i's (the last terms) will not change greatly the arguments presented in the case when p was equal to one. In the following we point out how our previous estimates can be extended for the case when p is larger than one.

The main feature of the perturbed systems in Section 4.3 is that their corresponding local free energy density have lower bounds that do not depend on the truncation parameter M. Since the extended local free energy just introduces non negative terms, we can define a similar truncation that maintains the same property, with such perturbed systems it is then possible to similarly establish Lemma 4.2.

As for Lemma 4.3, we treat the new terms by using the immersion of $H^1(\Omega)$ in $L^4(\Omega)$ and the estimates for the orientation field variables given in Lemma 4.2.

After we have extended the results of Lemmas 4.2 and 4.3, all the other lemmas are their direct consequence without any significative change due to the introduction of the new terms.

■

Bibliografia

[1] R. Dal Passo, L. Giacomelli, and A. Novick-Cohen. Existence for an Allen-Cahn/Cahn-Hilliard system with degenerate mobility. *Interfaces and Free Boundaries*, 1(2):199–226, 1999.

[2] C. Elliott and H. Garcke. On the Cahn-Hilliard equation with degenerate mobility. *SIAM Journal of Mathematical Analysis*, 27:404–423, 1996.

[3] Charles M. Elliott and Stefan Luckhaus. A generalised diffusion equation for phase separation of a multi-component mixture with interfacial free energy. Preprint 887, IMA (Minnesota), October 1991.

[4] Dan Fan, Long-Qing Chen, S.P. Chen, and Peter W. Voorhees. Phase field formulations for modelling the Ostwald ripening in two-phase systems. *Comp. Mater. Sci.*, 9:329–336, 1998.

[5] J.L. Lions. *Quelques méthodes de Résolution des Problèmes aux Limites non Linéaries.* Dunod, 1969.

Capítulo 5

Densidade de Energia Livre Limitada Inferiormente

Resumo

Analisamos um sistema de equações diferenciais parciais proposto por Fan, L.-Q. Chen, S. Chen e Voorhees no caso em que a densidade de energia livre local é limitada inferiormente. Tal sistema modela o fenômeno "Ostwald ripening" em sistemas bifásicos e acopla uma equação do tipo Cahn-Hilliard a várias equações do tipo Allen-Cahn. Provamos a existência e unicidade de uma solução fraca.

A Weak Solution of a Model for Ostwald Ripening

Patrícia Nunes da Silva
nunes@ime.unicamp.br

José Luiz Boldrini
boldrini@ime.unicamp.br

Abstract

We analyze a system of partial differential equations proposed by Fan, L.-Q. Chen, S. Chen and Voorhees in the case that the local free energy density has a lower bound. This system consists of a Cahn-Hilliard and several Allen-Cahn type equations and model Ostwald ripening in two-phase systems. We prove the existence and uniqueness of a weak solution.

5.1 Introduction

Ostwald ripening is a phenomenon observed in a wide variety of two-phase systems in which there is coarsening of one phase dispersed in the matrix of another. Because its practical importance, this process has been extensively studied in several degrees of generality. In particular for Ostwald ripening of anisotropic crystals, Fan et al. [4] presented a model taking in consideration both the evolution of the compositional field and of the crystallographic orientations.

Our objective in this paper is to do a mathematical analysis for a model of Ostwald ripening presented by Fan et al. [4] in the case that the local free energy density has a lower bound. Such model is constituted of the following Cahn-Hilliard and Allen-Cahn equations:

$$\begin{cases} \partial_t c = \nabla \cdot \left[D\nabla \left(\partial_c \mathcal{F} - \kappa_c \Delta c \right) \right], & (x,t) \in \Omega_T \\ \partial_t \theta_i = -L_i \left(\partial_{\theta_i} \mathcal{F} - \kappa_i \Delta \theta_i \right), & (x,t) \in \Omega_T \\ \partial_{\mathbf{n}} c = \partial_{\mathbf{n}} \left(\partial_c \mathcal{F} - \kappa_c \Delta c \right) = \partial_{\mathbf{n}} \theta_i = 0, & (x,t) \in S_T \\ c(x,0) = c_0(x), \quad \theta_i(x,0) = \theta_{i0}(x), & x \in \Omega \end{cases} \tag{5.1}$$

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for $i = 1, \dots, p$.

Here, Ω is the physical region where the Ostwald process is occurring; $\Omega_T = \Omega \times (0, T)$; $S_T = \partial\Omega \times (0, T)$; $0 < T < +\infty$; $\mathbf{n}$ denotes the unitary exterior normal vector and $\partial_{\mathbf{n}}$ is the exterior normal derivative at the boundary; $c(x,t)$, for $t \in [0,T]$, $0 < T < +\infty$, $x \in \Omega$, is the compositional field (fraction of the soluto with respect to the mixture); $\theta_i(x,t)$, for $i = 1, \dots, p$, are the crystallographic orientations fields; D, κ_c, L_i, κ_i are positive constants related to the material properties. The function $\mathcal{F} = \mathcal{F}(c, \theta_1, \dots, \theta_p)$ is the local free energy density which is given by

$$\begin{aligned}\mathcal{F}(c, \theta_1, \dots, \theta_p) &= -\frac{A}{2}(c - c_m)^2 + \frac{B}{4}(c - c_m)^4 + \frac{D_\alpha}{4}(c - c_\alpha)^4 \\ &+ \frac{D_\beta}{4}(c - c_\beta)^4 + \sum_{i=1}^{p}\left[-\frac{\gamma}{2}(c - c_\alpha)^2\theta_i^2 + \frac{\delta}{4}\theta_i^4\right] + \sum_{i=1}^{p}\sum_{i \neq j = 1}^{p}\frac{\varepsilon_{ij}}{2}\theta_i^2\theta_j^2;\end{aligned} \tag{5.2}$$

c_α and c_β are the solubilities in the matrix phase and the second phase respectively, and $c_m = (c_\alpha + c_\beta)/2$. The positive coefficients A, B, D_α, D_β, γ, δ and ε_{ij} are phenomenological parameters.

In this paper we obtain a unique $(p+1)$-tuple which is a weak solution to Problem (5.1) when local free energy density given in (5.2) is such that

$$\mathcal{F}(c, \theta_1, \dots, \theta_p) \geq m_{\mathcal{F}}, \qquad \forall c, \theta_1, \dots, \theta_p \in \mathbb{R}.$$

We remark that the above assumption is satisfied, for example, if there exists $E > 0$ such that $E(D_\alpha + D_\beta) - p\gamma$, $\delta - \gamma E > 0$.

Our approach to the problem is to analyze a family of suitable systems which approximate the model presented at (5.1). In this analysis, we show that the approximate solutions converge to a solution of the original model and this, in particular, will furnish a rigorous proof of the existence of weak solutions (see the statement of Theorem 5.1). Our approach uses an existence result presented by Passo et al. [1] for an Cahn-Hilliard/Allen-Cahn system with degenerate mobility.

Throughout this paper, standard notation will be used for the required functional spaces. We denote by $\overline{f}$ the mean value of f in Ω of a given $f \in L^1(\Omega)$.

5.2 Existence of Solutions

In this section we present our main result:

THEOREM 5.1 Let $T > 0$ and $\Omega \subset R^d$, $1 \leq d \leq 3$ be a bounded domain with Lipschitz boundary. For all c_0, θ_{i0}, $i = 1, \ldots, p$, satisfying c_0, $\theta_{i0} \in H^1(\Omega)$, there exists a unique $(p+1)$-tuple $(c, \theta_1, \ldots, \theta_p)$ such that, for $i = 1, \ldots, p$,
(a) $c \in L^\infty(0, T, H^1(\Omega)) \cap L^2(0, T, H^3(\Omega))$;
(b) $\theta_i \in L^\infty(0, T, H^1(\Omega)) \cap L^2(0, T, H^2(\Omega))$;
(c) $\partial_t c \in L^2(0, T, [H^1(\Omega)]')$, $\partial_t \theta_i \in L^2(\Omega_T)$;
(d) $\partial_c \mathcal{F}(c, \theta_1, \ldots, \theta_p)$, $\partial_{\theta_i} \mathcal{F}(c, \theta_1, \ldots, \theta_p) \in L^2(\Omega_T)$;
(e) $c(x, 0) = c_0(x)$, $\theta_i(x, 0) = \theta_{i0}(x)$;
(f) $\partial_{\mathbf{n}} c_{|S_T} = \partial_{\mathbf{n}} \theta_{i|S_T} = 0$ in $L^2(S_T)$;
(g) $(c, \theta_1, \ldots, \theta_p)$ satisfies

$$\int_0^T \langle \partial_t c, \phi \rangle dt = -\iint_{\Omega_T} D\nabla(\partial_c \mathcal{F}(c, \theta_1, \ldots, \theta_p) - \kappa_c \Delta c)\nabla\phi, \tag{5.3}$$

$\forall \phi \in L^2(0, T, H^1(\Omega))$ and

$$\iint_{\Omega_T} \partial_t \theta_i \psi_i = -\iint_{\Omega_T} L_i(\partial_{\theta_i} \mathcal{F}(c, \theta_1, \ldots, \theta_p) - \kappa_i \Delta\theta_i)\psi_i, \tag{5.4}$$

$\forall \psi_i \in L^2(\Omega_T), i = 1, \ldots, p$, and where $\mathcal{F}$ is given by (5.2), $\langle \cdot, \cdot \rangle$ denotes the duality pairing between $H^1(\Omega)$ and its dual and $(\cdot, \cdot)$ denotes the inner product in $L^2(\Omega)$.

The above uniqueness is proved below.

LEMMA 5.1 Under the hypotheses stated in Theorem 5.1, the $(p+1)$-tuple which solves (5.3)–(5.4) is uniquely determined.

Proof. We argue as Elliott and Luckhaus [3]. We introduce the Green's operator G: given $f \in [H^1(\Omega)]'_{null} = \{f \in [H^1(\Omega)]', \ \langle f, 1 \rangle = 0\}$, we define $Gf \in H^1(\Omega)$ as the unique solution of

$$\int_\Omega \nabla Gf \nabla\psi = \langle f, \psi \rangle, \quad \forall \psi \in H^1(\Omega) \qquad \text{and} \qquad \int_\Omega Gf = 0.$$

Let $z^c = c_1 - c_2$ and $z^{\theta_i} = \theta_{i1} - \theta_{i2}$, $i = 1, \ldots, p$, be the differences of two pair of solutions to (5.3)–(5.4) as in Theorem 5.1. Let

$$z^w = D[\partial_c \mathcal{F}(c_1, \theta_{11}, \ldots, \theta_{p1}) - \partial_c \mathcal{F}(c_2, \theta_{12}, \ldots, \theta_{p2}) - \kappa_c \Delta z^c].$$

Since equation (5.3) implies that the mean value of the composition field in Ω is conserved, we have that $(z^c, 1) = 0$ and we find from (5.3) that

$$-Gz_t^c = \overline{z^w}.$$

The definition of the Green operator and the fact that $(z^c, 1) = 0$ give

$$-(\nabla Gz_t^c, \nabla Gz^c) = -(Gz_t^c, z^c) = (\overline{z^w}, z^c) = (z^w, z^c).$$

Thus

$$\frac{1}{2}\frac{d}{dt}|\nabla Gz^c|^2 + (D[\partial_c\mathcal{F}(c_1, \theta_{11}, \dots, \theta_{p1}) - \partial_c\mathcal{F}(c_2, \theta_{12}, \dots, \theta_{p2}) - \kappa_c\Delta z^c], z^c) = 0.$$

We find from (5.4) that

$$\frac{D}{2L_i}\frac{d}{dt}|z^{\theta_i}|^2 + D\kappa_i|\nabla z^{\theta_i}|^2 + D\big(\partial_{\theta_i}\mathcal{F}(c_1, \theta_{11}, \dots, \theta_{p1}) - \partial_{\theta_i}\mathcal{F}(c_2, \theta_{12}, \dots, \theta_{p2}), z^{\theta_i}\big) = 0.$$

By adding the above equations, using the convexity of the function $[\mathcal{F} + H](c, \theta_1, \dots, \theta_p)$ with

$$H(c, \theta_1, \dots, \theta_p) = \frac{A}{2}(c - c_m)^2 + \frac{\gamma}{2}\sum_{i=1}^{p}(c - c_\alpha)^2\theta_i^2 - \sum_{i=1}^{p}\sum_{i\neq j=1}^{p}\frac{\varepsilon_{ij}}{2}\theta_i^2\theta_j^2,$$

and integrating by parts, we obtain

$$\begin{aligned}&\frac{1}{2}\frac{d}{dt}|\nabla \mathcal{G}z^c|^2 + \kappa_c D|\nabla z^c|^2 + \sum_{i=1}^{p}\left[\frac{D}{2L_i}\frac{d}{dt}|z^{\theta_i}|^2 + D\kappa_i|\nabla z^{\theta_i}|^2\right] \\ &\le \big(\nabla(H(c_1, \theta_{11}, \dots, \theta_{p1}) - H(c_2, \theta_{12}, \dots, \theta_{p2}))\cdot(z^c, z^{\theta_1}, \dots, z^{\theta_p}), 1\big).\end{aligned} \tag{5.5}$$

In order to estimate the term at the right hand side of the above inequality, we observe that since $c_j, \theta_{ij} \in L^\infty(0, T, H^1(\Omega))$, we have

$$\begin{aligned}&\gamma((c_1 - c_\alpha)\theta_{i1}^2 - (c_2 - c_\alpha)\theta_{i2}^2, z^c) = \gamma(z^c\theta_{i1}^2 + (c_2 - c_\alpha)(\theta_{i1}^2 - \theta_{i2}^2), z^c) \\ &\quad\le \frac{\kappa_c D}{4p}\|\nabla z^c\|_{L^2(\Omega)}^2 + \frac{D\kappa_i}{8p}\|\nabla z^{\theta_i}\|_{L^2(\Omega)}^2 + C\|z^{\theta_i}\|_{L^2(\Omega)}^2 + C\|z^c\|_{L^2(\Omega)}^2,\end{aligned}$$

$$\begin{aligned}&\gamma((c_1 - c_\alpha)^2\theta_{i1} - (c_2 - c_\alpha)^2\theta_{i2}, z^{\theta_i}) \\ &\quad\le \frac{\kappa_c D}{4p}\|\nabla z^c\|_{L^2(\Omega)}^2 + \frac{D\kappa_i}{8p}\|\nabla z^{\theta_i}\|_{L^2(\Omega)}^2 + C\|z^{\theta_i}\|_{L^2(\Omega)}^2 + C\|z^c\|_{L^2(\Omega)}^2,\end{aligned}$$

and

$$\varepsilon_{ij}(\theta_{i1}\theta_{j1}^2 - \theta_{i2}\theta_{j2}^2, z^{\theta_i}) = \varepsilon_{ij}(z^{\theta_i}\theta_{j1}^2 + \theta_{i2}(\theta_{j1}+\theta_{j2})(\theta_{j1}-\theta_{j2}), z^{\theta_i})$$
$$\leq \frac{D\kappa_i}{8(p-1)}\|\nabla z^{\theta_i}\|_{L^2(\Omega)}^2 + \frac{D\kappa_j}{8(p-1)}\|\nabla z^{\theta_j}\|_{L^2(\Omega)}^2 + C\|z^{\theta_i}\|_{L^2(\Omega)}^2 + C\|z^{\theta_j}\|_{L^2(\Omega)}^2.$$

The above inequalities together (5.5) imply that

$$\frac{1}{2}\frac{d}{dt}|\nabla \mathcal{G} z^c|^2 + \frac{\kappa_c D}{2}|\nabla z^c|^2 + \sum_{i=1}^{p}\left[\frac{D}{2L_i}\frac{d}{dt}|z^{\theta_i}|^2 + \frac{D\kappa_i}{2}|\nabla z^{\theta_i}|^2\right]$$
$$\leq C\left[\|z^c\|_{L^2(\Omega)}^2 + \sum_{i=1}^{p}\|z^{\theta_i}\|_{L^2(\Omega)}^2\right].$$

From the definition of the Green operator, we have that $|z^c|^2 = (\nabla\mathcal{G}z^c, \nabla z^c)$. Using the Hölder inequality, we can rewrite the above inequality as

$$\frac{1}{2}\frac{d}{dt}|\nabla \mathcal{G} z^c|^2 + \frac{\kappa_c D}{4}|\nabla z^c|^2 + \sum_{i=1}^{p}\left[\frac{D}{2L_i}\frac{d}{dt}|z^{\theta_i}|^2 + \frac{D\kappa_i}{2}|\nabla z^{\theta_i}|^2\right]$$
$$\leq C\left[\|\nabla\mathcal{G}z^c\|_{L^2(\Omega)}^2 + \sum_{i=1}^{p}\|z^{\theta_i}\|_{L^2(\Omega)}^2\right].$$

A standard Gronwall argument then yields uniqueness since

$$z^c(0) = 0 \qquad \text{and} \qquad z^{\theta_i}(0) = 0, \quad i = 1, \ldots, p.$$

■

To obtain the result in Theorem 5.1, we approximate system (5.1) by a family of suitable systems and then pass to the limit. In Section 5.3, we use the results of Passo et al. [1] to prove existence of solutions of such perturbed systems and to take the limit in these systems in the last sections.

For sake of simplicity of exposition, without loosing generality, we develop the proof for the case of dimension one and for only one orientation field variable, that is, when Ω is a bounded open interval and p is equal to one, and thus we have just one orientation field that we denote θ. In this case, the local free energy density is reduced to

$$\mathcal{F}(c,\theta) = -\frac{A}{2}(c-c_m)^2 + \frac{B}{4}(c-c_m)^4 + \frac{D_\alpha}{4}(c-c_\alpha)^4 + \frac{D_\beta}{4}(c-c_\beta)^4$$
$$-\frac{\gamma}{2}(c-c_\alpha)^2\theta^2 + \frac{\delta}{4}\theta^4. \tag{5.6}$$

Even though the crossed terms of (5.2) involving the orientation field variables are absent in above expression, when extending the result for p greater than one, they will not bring any difficulty as we point out at the end of the paper.

5.3 Perturbed Systems

In this section, we construct a family of perturbed systems. Such family depends on an auxiliary parameter M which controls a truncation of the local free energy $\mathcal{F}$ which will permit the application of an existence result of Passo et al. [1]. We consider

$$\mathcal{F}_M(c,\theta) = \mathcal{F}(c,\theta), \quad -M \le c,\theta \le M. \tag{5.7}$$

Outside the set $[-M,M]\times[-M,M]$, we extend the above function to satisfy

$$\|\partial_c\mathcal{F}_M\|_{C^1(\mathbf{R}^2,\mathbf{R})} \le U_0(M) \quad \text{and} \quad \|\partial_\theta\mathcal{F}_M\|_{C(\mathbf{R}^2,\mathbf{R})} \le V_0(M), \tag{5.8}$$

$$\begin{aligned} |\partial_c\mathcal{F}_M|^2 \le K[c^6+\theta^6+1] \quad &\text{and} \quad |\partial_{cc}\mathcal{F}_M|^2 \le K[c^4+\theta^4+1],\\ |\partial_\theta\mathcal{F}_M|^2 \le K[c^6+\theta^6+1] \quad &\text{and} \quad |\partial_{c\theta}\mathcal{F}_M|^2 \le K[c^4+\theta^4+1], \end{aligned} \tag{5.9}$$

$$|\mathcal{F}_M| \le K[c^4+\theta^4+1] \quad \text{and} \quad \mathcal{F}_M \ge m_{\mathcal{F}}, \tag{5.10}$$

$\forall M > 0$, $\forall c,\theta \in \mathbf{R}$, where $K > 0$ is a constant, $m_{\mathcal{F}}$ is a constant, and, for each M, $U_0(M)$ and $V_0(M)$ are also constants.

Remark. The above properties are not restrictive since they were already satisfied by the original energy density (5.6).

The perturbed systems are given by

$$\begin{cases} \partial_t c = D\left(\partial_c\mathcal{F}_M(c,\theta) - \kappa_c c_{xx}\right)_{xx}, & (x,t)\in\Omega_T\\ \partial_t\theta = -L\left[\partial_\theta\mathcal{F}_M(c,\theta) - \kappa\theta_{xx}\right], & (x,t)\in\Omega_T\\ \partial_{\mathbf{n}}c = \partial_{\mathbf{n}}(\partial_c\mathcal{F}_M(c,\theta) - \kappa_c c_{xx}) = \partial_{\mathbf{n}}\theta = 0, & (x,t)\in S_T\\ c(x,0) = c_0(x), \quad \theta(x,0) = \theta_0(x), & x\in\Omega \end{cases} \tag{5.11}$$

To solve the above problem, we shall use the next proposition which is an existence result stated by Passo et al. [1] to the following system:

$$\begin{cases} \partial_t u = \left[q_1(u,v)\left(f_1(u,v) - \kappa_1 u_{xx}\right)_x\right]_x, & (x,t) \in \Omega_T \\ \partial_t v = -q_2(u,v)\left[f_2(u,v) - \kappa_2 v_{xx}\right], & (x,t) \in \Omega_T \\ \partial_{\mathbf{n}} u = \partial_{\mathbf{n}} u_{xx} = \partial_{\mathbf{n}} v = 0, & (x,t) \in S_T \\ u(x,0) = u_0(x), \quad v(x,0) = v_0(x), & x \in \Omega \end{cases} \tag{5.12}$$

where q_i and f_i satisfy:
(H1) $q_i \in C(\mathbf{R}^2, \mathbf{R}^+)$, with $q_{\min} \leq q_i \leq q_{\max}$ for some $0 < q_{\min} \leq q_{\max}$;
(H2) $f_1 \in C^1(\mathbf{R}^2, \mathbf{R})$ and $f_2 \in C(\mathbf{R}^2, \mathbf{R})$, with $\|f_1\|_{C^1} + \|f_2\|_{C^0} \leq F_0$ for some $F_0 > 0$.

PROPOSITION 5.1 Assuming (H1), (H2) and $u_0,\ v_0 \in H^1(\Omega)$, there exists a pair of functions (u,v) such that:

(i). $u \in L^\infty(0,T,H^1(\Omega)) \cap L^2(0,T,H^3(\Omega)) \cap C([0,T];H^\lambda(\Omega))$, $\lambda < 1$

(ii). $v \in L^\infty(0,T,H^1(\Omega)) \cap L^2(0,T,H^2(\Omega)) \cap C([0,T];H^\lambda(\Omega))$, $\lambda < 1$

(iii). $\partial_t u \in L^2(0,T,[H^1(\Omega)]')$, $\quad \partial_t v \in L^2(\Omega_T)$

(iv). $u(0) = u_0$ and $v(0) = v_0$ in $L^2(\Omega)$

(v). $\partial_{\mathbf{n}} u_{|S_T} = \partial_{\mathbf{n}} v_{|S_T} = 0$ in $L^2(S_T)$

(vi). (u,v) solves (5.12) in the following sense:

$$\int_0^t \langle \partial_t u, \phi \rangle = -\iint_{\Omega_t} q_1(u,v)(f_1(u,v) - \kappa_1 u_{xx})_x \phi_x, \quad \forall \phi \in L^2(0,T,H^1(\Omega))$$
$$\iint_{\Omega_t} \partial_t v \psi = -\iint_{\Omega_t} q_2(u,v)(f_2(u,v) - \kappa_2 v_{xx})\psi, \quad \forall \psi \in L^2(\Omega_T).$$

REMARK. The regularity of the test functions with respect to t allow us to obtain the integrals over $(0,t)$, instead of $(0,T)$ as originally presented by Passo et al. [1].

Since (5.8) holds, applying the above proposition, for each $M > 0$ there exists a solution (c_M, θ_M) of Problem (5.11) in the following sense

$$\int_0^t \langle \partial_t c_M, \phi \rangle = -\iint_{\Omega_t} D(\partial_c \mathcal{F}_M(c_M,\theta_M) - \kappa_c [c_M]_{xx})_x \phi_x, \tag{5.13}$$

for $\phi \in L^2(0,T,H^1(\Omega))$ and

$$\iint_{\Omega_t} \partial_t \theta_M \psi = -\iint_{\Omega_t} L(\partial_\theta \mathcal{F}_M(c_M,\theta_M) - \kappa[\theta_M]_{xx})\psi, \tag{5.14}$$

for $\psi \in L^2(\Omega_T)$.

Let us observe that equation for c_M in equation (5.13) implies that the mean value of c_M in Ω is given by

$$\overline{c_M(t)} = \overline{c_0} \tag{5.15}$$

5.4 Limit as $M \to \infty$

In this section we obtain some a priori estimates that allow taking the limit in the parameter M.

LEMMA 5.2 There exists a constant C_1 independent of M (sufficiently large) such that

(i). $||c_M||_{L^\infty(0,T,H^1(\Omega))} \le C_1$

(ii). $||\theta_M||_{L^\infty(0,T,H^1(\Omega))} \le C_1$

(iii). $||(\partial_c \mathcal{F}_M - \kappa_c(c_M)_{xx})_x||_{L^2(\Omega_T)} \le C_1$

(iv). $||\partial_\theta \mathcal{F}_M - \kappa(\theta_M)_{xx}||_{L^2(\Omega_T)} \le C_1$

(v). $||\partial_t c_M||_{L^2(0,T,[H^1(\Omega)]')} \le C_1$

(vi). $||\partial_t \theta_M||_{L^2(\Omega_T)} \le C_1$

(vii). $||\mathcal{F}_M(c_M,\theta_M)||_{L^\infty(0,T,L^1(\Omega))} \le C_1$

Proof. To obtain items (iii), (iv) and (vii), we argue as Passo et al. [1] and Elliott and Garcke [2]. First, we observe that by the regularity of c_M and θ_M, we could take

$$\partial_c \mathcal{F}_M - \kappa_c(c_M)_{xx} \quad \text{and} \quad \partial_\theta \mathcal{F}_M - \kappa(\theta_M)_{xx}$$

as test functions in the equations (5.13) and (5.14), respectively, to obtain

$$
\begin{aligned}
&\int_0^t \langle \partial_t c_M, \partial_c \mathcal{F}_M - \kappa_c (c_M)_{xx} \rangle + \iint_{\Omega_t} \partial_t \theta_M \partial_\theta \mathcal{F}_M - \kappa(\theta_M)_{xx} \\
&= - \iint_{\Omega_t} D[(\partial_c \mathcal{F}_M - \kappa_c (c_M)_{xx})_x]^2 - \iint_{\Omega_t} L[\partial_\theta \mathcal{F}_M - \kappa(\theta_M)_{xx}]^2.
\end{aligned}
\tag{5.16}
$$

Also, given a small $h > 0$, we consider the functions

$$
\mathcal{F}_{Mh} = \mathcal{F}_M(c_{Mh}, \theta_M) \qquad \text{and} \qquad c_{Mh}(t, x) = \frac{1}{h} \int_{t-h}^{t} c_M(\tau, x) d\tau
$$

where we set $c_M(t, x) = c_0(x)$ for $t \leq 0$. Since $\partial_t c_{Mh}(t, x) \in L^2(\Omega_T)$, we have

$$
\begin{aligned}
&\int_0^t \langle (c_{Mh})_t, [\partial_c \mathcal{F}_{Mh} - \kappa_c (c_{Mh})_{xx}] \rangle dt + \iint_{\Omega_t} (\theta_M)_t [\partial_\theta \mathcal{F}_{Mh} - \kappa(\theta_M)_{xx}] \\
&= \int_\Omega \left[\frac{\kappa_c}{2} |[c_{Mh}(t)]_x|^2 + \frac{\kappa}{2} |[\theta_M]_x(t)|^2 + \mathcal{F}_{Mh}(t) \right] \\
&\qquad - \int_\Omega \left[\frac{\kappa_c}{2} |[c_0]_x|^2 + \frac{\kappa}{2} |[\theta_0]_x|^2 + \mathcal{F}_M(c_0, \theta_0) \right].
\end{aligned}
$$

Taking the limit as h tends to zero in the above expression and using (5.16), we obtain

$$
\begin{aligned}
&\iint_{\Omega_t} D[(\partial_c \mathcal{F}_M - \kappa_c (c_M)_{xx})_x]^2 + \iint_{\Omega_t} L[\partial_\theta \mathcal{F}_M - \kappa(\theta_M)_{xx}]^2 \\
&\qquad + \frac{\kappa_c}{2} \|[c_M]_x(t)\|^2_{L^2(\Omega)} + \frac{\kappa}{2} \|[\theta_M]_x(t)\|^2_{L^2(\Omega)} + \int_\Omega \mathcal{F}_M(t) \\
&= \frac{\kappa_c}{2} \|[c_0]_x\|^2_{L^2(\Omega)} + \frac{\kappa}{2} \|[\theta_0]_x\|^2_{L^2(\Omega)} + \int_\Omega \mathcal{F}_M(c_0, \theta_0)
\end{aligned}
$$

for almost every $t \in (0, T]$. Using the regularity of the initial conditions (see Theorem 5.1), (5.7) and (5.10), we could choose M_0, depending only on the initial conditions, to obtain for all $M > M_0$

$$
\begin{aligned}
&\iint_{\Omega_T} D[(\partial_c \mathcal{F}_M - \kappa_c (c_M)_{xx})_x]^2 + \iint_{\Omega_T} L[\partial_\theta \mathcal{F}_M - \kappa(\theta_M)_{xx}]^2 \\
&\qquad + \frac{\kappa_c}{2} \|[c_M]_x(t)\|^2_{L^2(\Omega)} + \frac{\kappa}{2} \|[\theta_M]_x(t)\|^2_{L^2(\Omega)} + \int_\Omega \mathcal{F}_M(t) \leq C_1
\end{aligned}
\tag{5.17}
$$

which implies items (iii), (iv) and (vii) since we have (5.10). Using the Poincaré inequality and (5.15), item (i) is also verified.

To prove item (vi), we choose $\psi = \partial_t \theta_M$ as a test function in (5.14), which yields

$$\begin{aligned}\iint_{\Omega_T} [\partial_t \theta_M]^2 &= -\iint_{\Omega_T} L(\partial_\theta \mathcal{F}_M - \kappa(\theta_M)_{xx})\partial_t \theta_M \\ &\leq \left(\iint_{\Omega_T} L^2(\partial_\theta \mathcal{F}_M - \kappa(\theta_M)_{xx})^2\right)^{1/2} \left(\iint_{\Omega_T} [\partial_t \theta_M]^2\right)^{1/2}.\end{aligned}$$

Since we have

$$\int_\Omega \theta_M^2 \leq 2\int_\Omega |\theta_0|^2 + 2t \iint_{\Omega_T} (\partial_t \theta_M)^2 d\tau \leq C_2,$$

item (vi) and (5.17), then item (ii) is verified. Finally, item (v) follows since

$$\left|\int_0^T \langle \partial_t c_M, \phi\rangle\right| \leq \left(\iint_{\Omega_T} D^2[(\partial_c \mathcal{F}_M - \kappa_c(c_M)_{xx})_x]^2\right)^{1/2} \left(\iint_{\Omega_T} (\phi_x)^2\right)^{1/2}$$

for all $\phi \in L^2(0, T, H^1(\Omega))$.

Remark. From (5.17), using (5.10), we obtain

$$\begin{aligned}\iint_{\Omega_T} D[(\partial_c \mathcal{F}_M - \kappa_c(c_M)_{xx})_x]^2 + \iint_{\Omega_T} L[\partial_\theta \mathcal{F}_M - \kappa(\theta_M)_{xx}]^2 \\ + \frac{\kappa_c}{2}\|[c_M(t)]_x\|^2_{L^2(\Omega)} + \frac{\kappa}{2}\|[\theta_M]_x(t)\|^2_{L^2(\Omega)} \leq C_1.\end{aligned}$$

Lemma 5.3 For M sufficiently large, there exist a constant C_3 independent of M such that

(i). $\|\partial_c \mathcal{F}_M\|_{L^2(0,T,H^1(\Omega))} \leq C_3$,

(ii). $\|\partial_\theta \mathcal{F}_M\|_{L^2(\Omega_T)} \leq C_3$,

(iii). $\|[c_M]_{xx}\|_{L^2(\Omega_T)} \leq C_3$,

(iv). $\|[\theta_M]_{xx}\|_{L^2(\Omega_T)} \leq C_3$, *Proof.* First, we prove items (ii) and (iv). From Lemma 5.2(iv), we have

$$\iint_{\Omega_T} (\partial_\theta \mathcal{F}_M)^2 - 2\kappa \iint_{\Omega_T} \partial_\theta \mathcal{F}_M [\theta_M]_{xx} + \kappa^2 \iint_{\Omega_T} [\theta_M]_{xx}^2 \leq C_3. \tag{5.18}$$

Using (5.9), we obtain

$$2\kappa \partial_\theta \mathcal{F}_M [\theta_M]_{xx} \leq \frac{\kappa^2}{2} [\theta_M]_{xx}^2 + C_3 [c_M^6 + \theta_M^6 + 1].$$

Thus, from Lemma 5.2(ii), it follows from (5.18) that

$$\iint_{\Omega_T} (\partial_\theta \mathcal{F}_M)^2 + \frac{\kappa^2}{2} \iint_{\Omega_T} [\theta_M]_{xx}^2 \leq C_3.$$

Now, we prove item (iii). Defining, $H_M = \partial_c \mathcal{F}_M - \kappa_c [c_M]_{xx}$, since $[c_M]_{x|S_T} = 0$, we have

$$\iint_{\Omega_T} H_M = \iint_{\Omega_T} \partial_c \mathcal{F}_M,$$

and from Lemma 5.2(iii),

$$\iint_{\Omega_T} [H_M]_x^2 \leq C_1.$$

We have

$$\iint_{\Omega_T} H_M^2 = \iint_{\Omega_T} (\partial_c \mathcal{F}_M)^2 - 2 \iint_{\Omega_T} (\partial_c \mathcal{F}_M)[c_M]_{xx} + \kappa_c^2 \iint_{\Omega_T} [c_M]_{xx}^2.$$

On the other hand, we can write

$$\iint_{\Omega_T} H_M^2 = \iint_{\Omega_T} [H_M - \overline{H_M}]^2 + \iint_{\Omega_T} \overline{H_M}^2 \leq C_P \iint_{\Omega_T} [H_M]_x^2 + \iint_{\Omega_T} (\partial_c \mathcal{F}_M)^2$$

where C_P denotes the Poincaré constant. Now, item (iii) follows from (5.9) and Lemma 5.2(i) and (ii).

Finally, using again (5.9) and Lemma 5.2(i) and (ii), we obtain

$$||\partial_c \mathcal{F}_M||_{L^2(\Omega_T)}^2 \leq C_3.$$

Lemma 5.2(i) and (ii) imply that $||[\partial_c \mathcal{F}_M]_x||_{L^2(\Omega_T)}^2$ is also bounded by a constant. Thus, we have proved the item (i).

We can now state the following result.

PROPOSITION 5.2 There exists a pair (c, θ) such that:

(i). $c \in L^\infty(0, T, H^1(\Omega)) \cap L^2(0, T, H^3(\Omega))$

(ii). $\theta \in L^\infty(0, T, H^1(\Omega)) \cap L^2(0, T, H^2(\Omega))$

(iii). $\partial_t c \in L^2(0, T, [H^1(\Omega)]')$, $\quad \partial_t \theta \in L^2(\Omega_T)$

(iv). $\partial_c \mathcal{F}(c, \theta)$, $\partial_\theta \mathcal{F}(c, \theta) \in L^2(\Omega_T)$

(v). $c(0) = c_0$ and $\theta(0) = \theta_0$ in $L^2(\Omega)$

(vi). $[c]_{x|S_T} = [\theta]_{x|S_T} = 0$ in $L^2(S_T)$

(vii). (c, θ) solves the perturbed system (5.11) in the following sense:

$$\int_0^T \langle \partial_t c, \phi \rangle = - \iint_{\Omega_T} D[\partial_c \mathcal{F}(c, \theta) - \kappa_c (c)_{xx}]_x \phi_x$$

for all $\phi \in L^2(0, T, H^1(\Omega))$, and

$$\iint_{\Omega_T} \partial_t \theta \psi = - \iint_{\Omega_T} L(\partial_\theta \mathcal{F}(c, \theta) - \kappa(\theta)_{xx})\psi$$

for all $\psi \in L^2(\Omega_T)$, and $\mathcal{F}$ is given by (5.6).

Proof. First, let us observe that from Lemma 5.2(iii) and Lemma 5.3(i), the norm of $[c_M]_{xxx}$ in $L^2(\Omega_T)$ is bounded by a constant which does not depend on M. This fact, the estimates of Lemmas 5.2 and 5.3 together with a compactness argument imply that there exists a subsequence (still denoted by $\{(c_M, \theta_M)\}$) that satisfies (as M goes to infinity)

$$\begin{aligned}
&c_M,\ \theta_M \quad \text{converge weakly-* to} \quad c, \theta \quad \text{in} \quad L^\infty(0, T, H^1(\Omega)),\\
&c_M, \quad \text{converges weakly to} \quad c \quad \text{in} \quad L^2(0, T, H^3(\Omega)),\\
&\theta_M, \quad \text{converges weakly to} \quad \theta \quad \text{in} \quad L^2(0, T, H^2(\Omega)),\\
&\partial_t c_M, \quad \text{converges weakly to} \quad \partial_t c \quad \text{in} \quad L^2(0, T, [H^1(\Omega)]'),\\
&\partial_t \theta_M, \quad \text{converges weakly to} \quad \partial_t \theta \quad \text{in} \quad L^2(\Omega_T)\\
&c_M,\ \theta_M \quad \text{converge to} \quad c, \theta \quad \text{in} \quad L^2(\Omega_T).
\end{aligned}$$

By recalling Lemmas 5.2 and 5.3, items (i)–(iii) now follow. Now, items (i) and (ii) of Lemma 5.3 imply that

$$\begin{aligned} \partial_c \mathcal{F}_M(c_M, \theta_M) &\quad \text{converges weakly to} \quad \mathcal{G} \quad \text{in} \quad L^2(\Omega_T), \\ \partial_\theta \mathcal{F}_M(c_M, \theta_M) &\quad \text{converges weakly to} \quad \mathcal{H} \quad \text{in} \quad L^2(\Omega_T). \end{aligned}$$

Since the strong convergence of the sequence (c_M) implies that (at least for a subsequence) $\partial_c \mathcal{F}_M(c_M, \theta_M)$ converges pointwise in Ω_T to $\partial_c \mathcal{F}(c, \theta)$, it follows from Lemma 1.3 from Lions [5], p. 12, that $\mathcal{G} = \partial_c \mathcal{F}(c, \theta)$. Similarly, we have $\mathcal{H} = \partial_\theta \mathcal{F}(c, \theta)$. Thus item (iv) is proved.

Item (v) is straightforward. Now, by compactness we have that

$$\begin{aligned} c_M &\quad \text{converges to} \quad c \quad \text{in} \quad L^2(0, T, H^{2-\rho}(\Omega)), \quad \rho > 0, \\ \theta_M &\quad \text{converges to} \quad \theta \quad \text{in} \quad L^2(0, T, H^{2-\rho}(\Omega)), \quad \rho > 0, \end{aligned}$$

which imply item (vi).

To prove item (vii), by using the previous convergences, we pass to the limit as M goes to infinity in the equations (5.13) and (5.14). Now, we complete the proof of Theorem 5.1. We argue that slight changes in the arguments previously presented prove the Theorem for higher spatial dimensions and $p > 1$.

Proof. Firstly, we discuss the case when the spatial dimension satisfies $d = 2, 3$. We start by remarking that, as observed by Passo et al. [1], Proposition 5.1 is valid for any dimension. Also, all of our previous arguments hold for dimensions $d = 2, 3$. In higher dimensions, we use an argument of elliptic regularity of the Laplacian to obtain estimates in $L^2(0, T, H^2(\Omega))$ and in $L^2(0, T, H^3(\Omega))$.

Now we explain the necessary modifications when the number of crystallographic orientations is larger than one. In this case, the local free energy density is given by

$$\begin{aligned} \mathcal{F}(c, \theta) = &- \frac{A}{2}(c - c_m)^2 + \frac{B}{4}(c - c_m)^4 + \frac{D_\alpha}{4}(c - c_\alpha)^4 + \frac{D_\beta}{4}(c - c_\beta)^4 \\ &- \frac{\gamma}{2} \sum_{i=1}^{p} \left[(c - c_\alpha)^2 \theta_i^2 + \frac{\delta}{4}\theta_i^4 + \sum_{i \neq j = 1}^{p} \frac{\varepsilon_{ij}}{2} \theta_i^2 \theta_j^2 \right]. \end{aligned}$$

Let us note that increasing the introduction of the mixed terms depending only on the θ_i's (the last terms) will not change greatly the arguments presented in the case when p was equal to one. In the following we point out how our previous estimates can be extended for the case when p is larger than one.

The main feature of the perturbed systems in Section 5.3 is that their corresponding local free energy density have lower bounds that do not depend on the truncation parameter M. Since the extended local free energy just introduces non negative terms, we can define a similar truncation that maintains the same property, with such perturbed systems it is then possible to similarly establish Lemma 5.2.

As for Lemma 5.3, we treat the new terms by using the immersion of $H^1(\Omega)$ in $L^4(\Omega)$ and the estimates for the orientation field variables given in Lemma 5.2.

After we have extended the results of Lemmas 5.2 and 5.3, all the other lemmas are their direct consequence without any significative change due to the introduction of the new terms. ■

Bibliografia

[1] R. Dal Passo, L. Giacomelli, and A. Novick-Cohen. Existence for an Allen-Cahn/Cahn-Hilliard system with degenerate mobility. *Interfaces and Free Boundaries*, 1(2):199–226, 1999.

[2] C. Elliott and H. Garcke. On the Cahn-Hilliard equation with degenerate mobility. *SIAM Journal of Mathematical Analysis*, 27:404–423, 1996.

[3] Charles M. Elliott and Stefan Luckhaus. A generalised diffusion equation for phase separation of a multi-component mixture with interfacial free energy. Preprint 887, IMA (Minnesota), October 1991.

[4] Dan Fan, Long-Qing Chen, S.P. Chen, and Peter W. Voorhees. Phase field formulations for modelling the Ostwald ripening in two-phase systems. *Comp. Mater. Sci.*, 9:329–336, 1998.

[5] J.L. Lions. *Quelques méthodes de Résolution des Problèmes aux Limites non Linéaries.* Dunod, 1969.

Conclusão

A maior dificuldade que encontramos no desenvolvimento deste trabalho foi devida ao fato da densidade de energia livre local associada ao sistema de equações diferenciais parciais proposto por Fan et al. [15] não ser limitada inferiormente. A limitação inferior da densidade de energia livre local é uma característica comumente presente em modelos envolvendo somente a equação de Cahn-Hilliard bem como em sistemas que acoplam equações do tipo Cahn-Hilliard e do tipo Allen-Cahn. Em nosso caso, a falta de limitação é devida essencialmente aos termos, presentes na função $\mathcal{F}$, que acoplam a variável de campo associada à concentração e as variáveis associadas às orientações cristalográficas.

A fim de contornar tal dificuldade e baseados nas observações feitas nos artigos sobre as propriedades da função $\mathcal{F}$, propusemos, no Capítulo 1, uma família de sistemas relacionados ao sistema proposto originalmente por Fan et al. [15]. Em tal família, a função $\mathcal{F}$ satisfaz as propriedades citadas e há exemplos cujas respectivas funções $\mathcal{F}$ coincidem em uma bola com a $\mathcal{F}$ proposta no modelo original. Para esta família obtivemos um resultado de existência e unicidade de uma solução fraca. Ainda para esta família, no Capítulo 3, melhoramos a regularidade da solução fraca.

No Capítulo 2, obtivemos existência e unicidade de uma solução generalizada para o modelo proposto por Fan et al. [15]; neste caso, obtivemos uma estimativa L^∞ no espaço e no tempo para componente associada a concentração. Tal estimativa satisfaz uma exigência física de que a concentração assuma valores em um intervalo fechado determinado por valores associados ao modelo.

Ainda com o objetivo de limitar inferiomente o funcional de energia associado ao sistema, no Capítulo 4, apresentamos uma nova família de sistemas em que modificamos a ordem dos termos que acoplam a variável de campo associada à concentração e as variáveis associadas às orientações cristalográficas. Para tal família apresentamos resultados de existência e unicidade de solução com a mesma regularidade da solução obtida no Capítulo 3.

Para efeito de completude, no Capítulo 5, apresentamos resultados de existência e unicidade de solução para o modelo proposto por Fan et al. [15] em um caso especial em que temos a limitação da densidade de energia livre local associada ao sistema. Obtivemos existência e unicidade de uma solução fraca.

Em termos de trabalhos futuros, pretendemos estudar o comportamento assintótico das soluções obtidas bem como prosseguir o estudo destes sistemas incorporando efeitos convectivos.

Bibliografia

[1] F. Bernis and A. Friedman. Higher order nonlinear degenerate parabolic equations. *Journal of Differential Equations*, 83:179–206, 1990.

[2] G. Caginalp. An analysis of a phase filed of a free boundary. *Arch. Rat. Mech. Anal.*, 92:205–245, 1986.

[3] G. Caginalp and E. A. Socolovsky. Computation of sharp phase boundaries by spreading the planar and spherically symmetric cases. *J. Comp. Phys.*, 1:85–100, 1991.

[4] J. W. Cahn and Hilliard J. E. Spinodal decomposition – a reprise. *Acta Metall.*, 19:151–161, 1971.

[5] J. W. Cahn and A. Novick-Cohen. Evolution equations for phase separation and ordering in binary alloys. *J. Stat. Phys.*, 76:877–909, 1992.

[6] J.C. Cahn and J. E. Hilliard. Free energy of a non-uniform system. I. Interfacial free energy. *Journal of Chemical Physics*, 28:258–267, 1958.

[7] Long-Qing Chen and Dan Fan. Computer simulation for a coupled grain growth and Ostwald ripening–application to Al_2O_3–Zr_2 two-phase systems. *J. Amer. Ceram. Soc.*, 79(5):1163–1168, 1996.

[8] Long-Qing Chen and Dan Fan. Computer simulation of grain growth using a continuum filed model. *Acta Mater.*, 45(2):611–622, 1997.

[9] Long-Qing Chen and Dan Fan. Diffusion-controlled grain growth in two-phase solids. *Acta Mater.*, 45(8):3297–3310, 1997.

[10] Long-Qing Chen, Dan Fan, and Chengwei Geng. Computer simulation of topological evolution in 2-d grain growth using a continuum diffusion-interface filed model. *Acta Mater.*, 45(3):1115–1126, 1997.

[11] M. I. M. Copetti and Charles M. Elliott. Numerical analysis of the Cahn-Hilliard equation with a logarithmic free energy. *Numer. Math.*, 63:39–65, 1992.

[12] R. Dal Passo, L. Giacomelli, and A. Novick-Cohen. Existence for an Allen-Cahn/Cahn-Hilliard system with degenerate mobility. *Interfaces and Free Boundaries*, 1(2):199–226, 1999.

[13] C. Elliott and H. Garcke. On the Cahn-Hilliard equation with degenerate mobility. *SIAM Journal of Mathematical Analysis*, 27:404–423, 1996.

[14] Charles M. Elliott and Stefan Luckhaus. A generalised diffusion equation for phase separation of a multi-component mixture with interfacial free energy. Preprint 887, IMA (Minnesota), October 1991.

[15] Dan Fan, Long-Qing Chen, S.P. Chen, and Peter W. Voorhees. Phase field formulations for modelling the Ostwald ripening in two-phase systems. *Comp. Mater. Sci.*, 9:329–336, 1998.

[16] J. S. Langer. *Models of pattern formation in first-order phase transitions.* Edgard Blücher LTDA, 1986.

[17] J.L. Lions. *Quelques méthodes de Résolution des Problèmes aux Limites non Linéaries.* Dunod, 1969.

[18] N. Tavare. *Industrial Cristalization, Process Simulation, Analysis and Design.* Plenum Press, 1995.