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A CAHN–HILLIARD MODEL BASED ON MICROCONCENTRATIONS

SAMUEL FOREST¹, ALAIN MIRANVILLE²

ABSTRACT. Our aim in this paper is to study a Cahn–Hilliard type system based on microconcentrations. We prove the existence and uniqueness of solutions to this system and then prove the convergence of the solutions to those of the original Cahn–Hilliard equation as a small parameter goes to zero, on finite time intervals.

1. INTRODUCTION

The Cahn–Hilliard equation is a fundamental equation in materials science and describes phase separation processes in binary alloys (see [1], [2] and [12]). More precisely, it describes the rapid separation of phases in a binary alloy (one speaks of spinodal decomposition and coarsening). We refer the interested reader to [10] for a review on the mathematical analysis of this equation, as well as several of its variants.

We can note that the original derivation of the Cahn–Hilliard equation essentially is phenomenological. As a consequence, several approaches were proposed to derive this equation or proper approximated models. We can mention in particular [4], [8], [11] and [13].

An extension of the Cahn–Hilliard model was proposed in [15] involving a nonlocal concentration variable in addition to the standard concentration. It was motivated by a free energy potential, proposed in earlier literature, with long-range interactions between particles in the form of a kernel function defined in a finite region around the material point. The fully nonlocal theory was replaced by a differential form in which the additional concentration is solution to a Helmholtz-type equation coupled with the standard concentration. The nonlocal concentration variable was interpreted as a weighted average of the standard concentration over a finite neighbourhood. This nonlocal formulation was also used in [16] for phase changes in electrode particles of lithium-ion batteries.

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The theory was reinterpreted in [7] in terms of a quadratic free energy density functional involving the difference between the local and nonlocal concentrations and the gradient of the nonlocal concentration. The additional concentration variable was called microconcentration referring to micro-continuum theories initiated by Eringen [5]. In Eringen's micromorphic continuum theory for instance, a microdeformation variable is introduced in addition to the standard deformation and the difference between micro and macro-deformations is penalized in the free energy density functional. Similarly, the free energy potential in [7] includes the square of the norm of the microconcentration gradient and the square of the difference between micro and standard concentrations. The coefficient in front of the last term can be interpreted as a penalty modulus. It was suggested in [7] that the microconcentration field converges to the solution to the Cahn–Hilliard equation for large values of the penalty modulus. No actual proof of this conjecture was however provided in [7].

The microconcentration model was further used in [3] in an application to lithium-ion batteries, coupled with finite deformation elastoplasticity. The computational advantage of the microconcentration approach, compared to the standard Cahn–Hilliard model, is that less regularity of shape functions is required for the concentration variables in a finite element setting [9].

Our aim in this paper is to prove the aforementioned convergence. We also prove the existence of solutions to the Cahn–Hilliard model based on microconcentrations and obtain error estimates on the difference of the solutions to this model and the original Cahn–Hilliard equation, on finite time intervals.

2. SETTING OF THE PROBLEM AND NOTATION

We consider the following initial and boundary value problem in a bounded and regular domain Ω of \mathbb{R}^n , $n = 1, 2$ or 3 , with boundary Γ :

$$(2.1) \quad \frac{\partial u}{\partial t} + \Delta^2 v - \Delta f(u) = 0,$$

$$(2.2) \quad u = v - \varepsilon \Delta v,$$

$$(2.3) \quad \frac{\partial u}{\partial \nu} = \frac{\partial v}{\partial \nu} = \frac{\partial \Delta v}{\partial \nu} = 0 \text{ on } \Gamma,$$

$$(2.4) \quad u|_{t=0} = u_0,$$

where ν is the unit outer normal to Γ and $\frac{\partial w}{\partial \nu} = \nabla w \cdot \nu$ denotes the normal derivative on Γ . Furthermore, $\varepsilon > 0$ is expected to be small (it is related to the inverse of the penalty modulus mentioned in the introduction); in particular, we assume, throughout this paper, that

$$(2.5) \quad 0 < \varepsilon \leq \varepsilon_0 < 1.$$

Finally, we take, for simplicity, $f(s) = s^3 - s$ and note that $f' \geq -1$.

Remark 2.1. In the above equations, u is the order parameter, while v is the microconcentration. In particular, in the presence of the microconcentration, the total (Ginzburg–Landau type) free energy associated with the problem reads (see [7])

$$\Psi(u, v, \nabla v) = \int_{\Omega} \left(\frac{1}{2\varepsilon} (u - v)^2 + \frac{1}{2} |\nabla v|^2 + F(u) \right) dx,$$

where the potential F is such that $F' = f$. Proceeding as in the classical Cahn–Hilliard theory, the chemical potential μ is then defined as a variational derivative of the free energy with respect to u , yielding, in view of the definition (2.2) of the microconcentration,

$$\mu = \frac{1}{\varepsilon} (u - v) + f(u) = -\Delta v + f(u).$$

We thus see that both u and v enter the definition of the chemical potential. Furthermore, when $\varepsilon = 0$, i.e., in the absence of the microconcentration, then we (formally) have $u = v$ and we recover the classical Cahn–Hilliard framework.

We set, for $w \in L^1(\Omega)$,

$$\langle w \rangle = \frac{1}{\text{Vol}(\Omega)} \int_{\Omega} w(x) dx$$

and, for $w \in H^1(\Omega)'$,

$$\langle w \rangle = \frac{1}{\text{Vol}(\Omega)} \langle w, 1 \rangle_{H^1(\Omega)', H^1(\Omega)},$$

where $\langle \cdot, \cdot \rangle$ denotes the duality product. Furthermore, we set, whenever it makes sense,

$$\bar{w} = w - \langle w \rangle.$$

Integrating (formally) (2.1) over Ω , we have, owing to (2.3),

$$(2.6) \quad \frac{d}{dt} \langle u \rangle = 0.$$

Integrating then (again formally) (2.2) over Ω , we obtain

$$(2.7) \quad \langle u \rangle = \langle v \rangle,$$

so that, also,

$$(2.8) \quad \frac{d}{dt} \langle v \rangle = 0.$$

We thus have the conservation of mass, both for the concentration u and the micro-concentration v .

Let A be the operator defined by

$$\langle Au, w \rangle_{H^1(\Omega)', H^1(\Omega)} = ((\nabla u, \nabla w)), \quad \forall w \in \bar{H}^1(\Omega),$$

for u given in $\bar{H}^1(\Omega)$, where $((\cdot, \cdot))$ denotes the usual L^2 -scalar product, with associated norm $\|\cdot\|$, and

$$\bar{H}^1(\Omega) = \{w \in H^1(\Omega), \langle w \rangle = 0\}.$$

We also set

$$\bar{L}^2(\Omega) = \{w \in L^2(\Omega), \langle w \rangle = 0\}.$$

The operator A is an unbounded linear, selfadjoint and positive operator with compact inverse and is an isomorphism from $\bar{H}^1(\Omega)$ onto its dual. Furthermore,

$$D(A) = \{w \in H^2(\Omega) \cap \bar{H}^1(\Omega), \frac{\partial w}{\partial \nu} = 0 \text{ on } \Gamma\}$$

and $Au = h$, $u \in D(A)$, $h \in \bar{L}^2(\Omega)$, is equivalent to

$$-\Delta u = h, \quad \frac{\partial u}{\partial \nu} = 0 \text{ on } \Gamma.$$

We will thus write $-\Delta$ instead of A in what follows, meaning that we consider that this operator acts on functions with null spatial average; of course, it can also be defined on functions with nonvanishing spatial average. We refer the interested reader to, e.g., [10] for more details on this.

Having this, we can rewrite, equivalently, (2.1) in the (weaker) form

$$(2.9) \quad (-\Delta)^{-1} \frac{\partial u}{\partial t} - \Delta v + \overline{f(u)} = 0,$$

noting that $\langle \frac{\partial u}{\partial t} \rangle = 0$. Considering (2.9) instead of (2.1), we only keep one boundary condition on v , namely,

$$(2.10) \quad \frac{\partial v}{\partial \nu} = 0 \text{ on } \Gamma.$$

Remark 2.2. Note that it follows from (2.1)-(2.2) that

$$(2.11) \quad \frac{\partial}{\partial t}(v - \varepsilon \Delta v) + \Delta^2 v - \Delta f(v - \varepsilon \Delta v) = 0,$$

which we can rewrite in the equivalent weaker form

$$(2.12) \quad \frac{\partial}{\partial t}((- \Delta)^{-1} \bar{v} + \varepsilon \bar{v}) - \Delta \bar{v} + \overline{f(\langle u_0 \rangle + \bar{v} - \varepsilon \Delta \bar{v})} = 0,$$

where we emphasize that $- \Delta$ acts on functions with null spatial average. Also recall that

$$\langle u \rangle = \langle v \rangle = \langle u_0 \rangle, \quad t \geq 0.$$

Alternatively, we can rewrite (2.2) in the equivalent form

$$(2.13) \quad \langle v \rangle = \langle u_0 \rangle, \quad \bar{v} = (I - \varepsilon \Delta)^{-1} \bar{u},$$

allowing us to rewrite (2.9) in the equivalent form

$$(2.14) \quad (- \Delta)^{-1} \frac{\partial \bar{u}}{\partial t} - \Delta (I - \varepsilon \Delta)^{-1} \bar{u} + \overline{f(\langle u_0 \rangle + \bar{u})} = 0.$$

This shows that we can rewrite (2.1)-(2.4) as an equivalent problem for the sole unknown u (resp., v).

We set $\| \cdot \|_{-1} = \| (- \Delta)^{-\frac{1}{2}} \cdot \|$; $\| \cdot \|_{-1}$ is a norm on $\{v \in H^1(\Omega)', \langle v \rangle = 0\}$ which is equivalent to the usual $H^1(\Omega)'$ -norm. More generally, we denote by $\| \cdot \|_X$ the norm on the Banach space X .

Throughout this paper, the same letters c and c' denote (nonnegative or positive) constants which may vary from line to line, or even in a same line, and which are independent of ε (but may depend on ε_0).

3. A PRIORI ESTIMATES

The estimates below are formal, but can be justified within a proper Galerkin scheme (see Section 4).

Multiplying (2.9) by $\frac{\partial u}{\partial t}$ and integrating over Ω and by parts, we have, recalling that $\langle \frac{\partial u}{\partial t} \rangle = 0$,

$$\frac{d}{dt} \int_{\Omega} F(u) dx - ((\Delta v, \frac{\partial u}{\partial t})) + \|\frac{\partial u}{\partial t}\|_{-1}^2 = 0,$$

where $F(s) = \int_0^s f(\xi) d\xi$. Noting that it follows from (2.2) that

$$(3.1) \quad \frac{\partial u}{\partial t} = \frac{\partial v}{\partial t} - \varepsilon \Delta \frac{\partial v}{\partial t},$$

we obtain

$$(3.2) \quad \frac{d}{dt} (\|\nabla v\|^2 + \varepsilon \|\Delta v\|^2 + 2 \int_{\Omega} F(u) dx) + 2 \|\frac{\partial u}{\partial t}\|_{-1}^2 = 0.$$

This yields the decay of the total free energy, together with estimates on u in $L^\infty(\mathbb{R}^+; L^4(\Omega))$, on v in $L^\infty(\mathbb{R}^+; H^2(\Omega))$ and on $\frac{\partial u}{\partial t}$ in $L^2(\mathbb{R}^+; H^1(\Omega)')$. Note indeed that it follows from Young's inequality that

$$F(s) = \frac{1}{4}s^4 - \frac{1}{2}s^2 \geq \frac{1}{8}s^4 - c.$$

It also follows from (3.1) that $\frac{\partial v}{\partial t}$ belongs to $L^2(\mathbb{R}^+; H^1(\Omega))$, noting that $\frac{\partial}{\partial v} \frac{\partial v}{\partial t} = 0$ on Γ . Furthermore, the estimates on u and $\frac{\partial u}{\partial t}$ are uniform with respect to ε , owing to (2.5), while only the estimate on v in $L^\infty(\mathbb{R}^+; H^1(\Omega))$ is uniform. Note however that $\varepsilon^{\frac{1}{2}}v$ is bounded, uniformly with respect to ε , in $L^\infty(\mathbb{R}^+; H^2(\Omega))$.

Remark 3.1. Recall that, when $\varepsilon = 0$, then (formally) $v = u$ and (3.2) reads

$$(3.3) \quad \frac{d}{dt} (\|\nabla u\|^2 + 2 \int_{\Omega} F(u) dx) + 2 \|\frac{\partial u}{\partial t}\|_{-1}^2 = 0,$$

which is precisely the energy decay for the original Cahn–Hilliard equation.

We next multiply (2.9) by $-\Delta u$ and find, recalling that $f' \geq -1$,

$$(3.4) \quad \frac{1}{2} \frac{d}{dt} \|u\|^2 + ((\Delta u, \Delta v)) \leq \|\nabla u\|^2.$$

Noting that $-\Delta v = \frac{1}{\varepsilon}(u - v)$, we have

$$(3.5) \quad \frac{1}{2} \frac{d}{dt} \|u\|^2 + \frac{1}{\varepsilon} \|\nabla u\|^2 \leq \|\nabla u\|^2 + \frac{1}{\varepsilon} ((\nabla u, \nabla v)).$$

Writing, employing Young's inequality,

$$\frac{1}{\varepsilon} |((\nabla u, \nabla v))| \leq \frac{1}{\varepsilon} \|\nabla u\| \|\nabla v\|$$

$$\leq \frac{1}{2} \left(\frac{1}{\varepsilon} - 1 \right) \|\nabla u\|^2 + \frac{1}{2\varepsilon(1-\varepsilon)} \|\nabla v\|^2,$$

we find

$$(3.6) \quad \frac{d}{dt} \|u\|^2 + \left(\frac{1}{\varepsilon} - 1 \right) \|\nabla u\|^2 \leq \frac{1}{\varepsilon(1-\varepsilon)} \|\nabla v\|^2,$$

which yields

$$(3.7) \quad \frac{d}{dt} (\varepsilon \|u\|^2) + (1 - \varepsilon_0) \|\nabla u\|^2 \leq \frac{1}{1 - \varepsilon_0} \|\nabla v\|^2.$$

This gives, in view of (2.5), an estimate on u in $L^2(0, T; H^1(\Omega))$, $T > 0$ given, which is uniform with respect to ε . Writing now, in view of (2.2),

$$\Delta u = \Delta v - \varepsilon \Delta^2 v,$$

we deduce from (3.4) that

$$(3.8) \quad \frac{d}{dt} \|u\|^2 + \|\Delta v\|^2 + \varepsilon \|\nabla \Delta v\|^2 \leq 2 \|\nabla u\|^2,$$

which gives an estimate on v in $L^2(0, T; H^3(\Omega))$; this estimate is not uniform with respect to ε . However, $\varepsilon^{\frac{1}{2}} v$ is bounded, uniformly with respect to ε , in this space and we have a uniform (with respect to ε) estimate on v in $L^2(0, T; H^2(\Omega))$.

4. EXISTENCE AND UNIQUENESS OF SOLUTIONS

We consider the initial and boundary value problem

$$(4.1) \quad (-\Delta)^{-1} \frac{\partial \bar{u}}{\partial t} - \Delta \bar{v} + \overline{f(\langle u_0 \rangle + \bar{u})} = 0,$$

$$(4.2) \quad \langle u \rangle = \langle v \rangle = \langle u_0 \rangle, \quad t \geq 0,$$

$$(4.3) \quad \bar{u} = \bar{v} - \varepsilon \Delta \bar{v},$$

$$(4.4) \quad \frac{\partial \bar{v}}{\partial \nu} = 0 \text{ on } \Gamma,$$

$$(4.5) \quad u|_{t=0} = u_0,$$

where $u = \langle u_0 \rangle + \bar{u}$ and $v = \langle u_0 \rangle + \bar{v}$, which we rewrite, equivalently, as

$$(4.6) \quad \frac{\partial}{\partial t} ((-\Delta)^{-1} \bar{v} + \varepsilon \bar{v}) - \Delta \bar{v} + \overline{f(\langle u_0 \rangle + \bar{v} - \varepsilon \Delta \bar{v})} = 0,$$

$$(4.7) \quad \langle u \rangle = \langle v \rangle = \langle u_0 \rangle, \quad t \geq 0,$$

$$(4.8) \quad \bar{u} = \bar{v} - \varepsilon \Delta \bar{v},$$

$$(4.9) \quad \frac{\partial \bar{v}}{\partial \nu} = 0 \text{ on } \Gamma,$$

$$(4.10) \quad u|_{t=0} = u_0,$$

where, again, $u = \langle u_0 \rangle + \bar{u}$ and $v = \langle u_0 \rangle + \bar{v}$

We have the following.

Theorem 4.1. *We assume that (2.5) holds and that $u_0 \in H^1(\Omega)$ and $\varepsilon u_0 \in H^2(\Omega)$. Then (4.1)-(4.5) possesses a unique weak solution (u, v) such that, $\forall T > 0$,*

$$\begin{aligned} u &\in L^\infty(\mathbb{R}^+; L^4(\Omega)) \cap L^2(0, T; H^1(\Omega)), \\ \frac{\partial u}{\partial t} &\in L^2(\mathbb{R}^+; H^1(\Omega)'), \\ v &\in L^\infty(\mathbb{R}^+; H^2(\Omega)) \cap L^2(0, T; H^3(\Omega)), \end{aligned}$$

$$\frac{\partial v}{\partial t} \in L^2(\mathbb{R}^+; H^1(\Omega)).$$

Furthermore, $u \in \mathcal{C}([0, T]; L^4(\Omega)_w)$ and $v \in C([0, T]; H^2(\Omega))$, where the index w denotes the weak topology.

Remark 4.2. Note that when we will pass to the limit below, we will no longer need, at the limit, $u_0 \in H^2(\Omega)$. However, we will still need $u_0 \in H^1(\Omega)$, since (3.2) formally reduces to (3.3) at the limit.

Proof. Uniqueness:

Let (u_1, v_1) and (u_2, v_2) be two solutions with initial data $u_{1,0}$ and $u_{2,0}$, respectively, such that $\langle u_{1,0} \rangle = \langle u_{2,0} \rangle$. We set $(u, v) = (u_1, v_1) - (u_2, v_2)$ and $u_0 = u_{1,0} - u_{2,0}$. Then, (u, v) solves

$$(4.11) \quad (-\Delta)^{-1} \frac{\partial u}{\partial t} - \Delta v + \overline{f(u_1)} - \overline{f(u_2)} = 0,$$

$$(4.12) \quad u = v - \varepsilon \Delta v,$$

$$(4.13) \quad \langle u \rangle = \langle v \rangle = 0, \quad t \geq 0,$$

$$(4.14) \quad \frac{\partial v}{\partial \nu} = 0 \text{ on } \Gamma,$$

$$(4.15) \quad u|_{t=0} = u_0.$$

We multiply (4.11) by u and have, recalling that $f' \geq -1$,

$$(4.16) \quad \frac{1}{2} \frac{d}{dt} \|u\|_{-1}^2 + ((u, -\Delta v)) \leq \|u\|^2.$$

Note that it follows from (4.12) that

$$((u, -\Delta v)) = \|\nabla v\|^2 + \varepsilon \|\Delta v\|^2$$

and

$$\|u\|^2 = \|v\|^2 + 2\varepsilon \|\nabla v\|^2 + \varepsilon^2 \|\Delta v\|^2.$$

We thus deduce that

$$\frac{1}{2} \frac{d}{dt} \|u\|_{-1}^2 + \|\nabla v\|^2 + \varepsilon \|\Delta v\|^2 \leq \|v\|^2 + 2\varepsilon \|\nabla v\|^2 + \varepsilon^2 \|\Delta v\|^2$$

and (2.5) yields, employing the Poincaré–Wirtinger inequality,

$$(4.17) \quad \frac{d}{dt} \|u\|_{-1}^2 + (1 - \varepsilon_0)\varepsilon \|\Delta v\|^2 \leq c \|\nabla v\|^2.$$

Writing next

$$\begin{aligned} \|u\|_{-1}^2 &= \|(-\Delta)^{-\frac{1}{2}}(v - \varepsilon \Delta v)\|^2 \\ &= \|v\|_{-1}^2 + 2\varepsilon \|v\|^2 + \varepsilon^2 \|\nabla v\|^2, \end{aligned}$$

it follows that

$$(4.18) \quad \frac{d}{dt} \|u\|_{-1}^2 \leq \frac{c}{\varepsilon^2} \|u\|_{-1}^2.$$

Gronwall's lemma finally yields the continuous (with respect to the $H^1(\Omega)'$ -norm) dependence on the initial data, as well as the uniqueness, for u . The uniqueness for v follows.

Existence:

Let $(w_i)_{i \in \mathbb{N}}$ be an orthonormal in $\bar{L}^2(\Omega)$ and orthogonal in $\bar{H}^1(\Omega)$ basis formed of eigenvectors of the operator $-\Delta$ associated with Neumann boundary conditions

and acting on functions with null spatial average. We call $0 < \lambda_1 \leq \lambda_2 \leq \dots$ the associated eigenvectors and set $W_m = \text{Span}\{w_1, \dots, w_m\}$.

We look, setting $w_0 = \frac{1}{\text{Vol}(\Omega)^{\frac{1}{2}}}$, for

$$\begin{aligned} v_m &= c_0 w_0 + \bar{v}_m, \quad c_0 = \text{Vol}(\Omega)^{\frac{1}{2}} \langle u_0 \rangle, \\ \bar{v}_m &= \sum_{i=1}^m c_{i,m} w_m, \end{aligned}$$

such that

$$(4.19) \quad \frac{d}{dt}(((-\Delta)^{-1} \bar{v}_m + \varepsilon \bar{v}_m, w)) + ((\nabla \bar{v}_m, \nabla w)) + ((f(\langle u_0 \rangle + \bar{v}_m - \varepsilon \Delta \bar{v}_m), w)) = 0,$$

$$\forall w \in W_m,$$

$$(4.20) \quad \bar{v}_m|_{t=0} = \bar{v}_{0,m},$$

where

$$(4.21) \quad \bar{v}_{0,m} - \varepsilon \Delta \bar{v}_{0,m} = \bar{u}_{0,m},$$

$$(4.22) \quad \bar{u}_{0,m} = P_m \bar{u}_0,$$

P_m being the orthogonal projector onto W_m (for the $L^2(\Omega)$ -norm). This means that

$$(4.23) \quad \bar{u}_{0,m} = \sum_{i=1}^m ((u_0, w_i)) w_i$$

and, if

$$(4.24) \quad \bar{v}_{0,m} = \sum_{i=1}^m d_i w_i,$$

then it follows from (4.21) that

$$\sum_{i=1}^m (1 + \varepsilon \lambda_i) d_i w_i = \sum_{i=1}^m ((u_0, w_i)) w_i,$$

so that

$$(4.25) \quad d_i = \frac{1}{1 + \varepsilon \lambda_i} ((u_0, w_i)), \quad i = 1, \dots, m.$$

Finally, having solved (4.19)-(4.20), we set

$$(4.26) \quad u_m = \langle u_0 \rangle + \bar{u}_m,$$

$$(4.27) \quad \bar{u}_m = \bar{v}_m - \varepsilon \Delta \bar{v}_m,$$

meaning that

$$(4.28) \quad \bar{u}_m = \sum_{i=1}^m (1 + \varepsilon \lambda_i) c_{i,m} w_i.$$

Now, taking $w = w_i$ in (4.19), we have

$$(4.29) \quad \left(\frac{1}{\lambda_i} + \varepsilon \right) c'_{i,m} + \lambda_i c_{i,m} + g_i(C) = 0,$$

$$(4.30) \quad c_{i,m}(0) = \frac{1}{1 + \varepsilon \lambda_i} ((\bar{u}_0, w_i)),$$

$i = 1, \dots, m$, where

$$C = \begin{pmatrix} c_{1,m} \\ \vdots \\ c_{m,m} \end{pmatrix}, \quad g(C) = \begin{pmatrix} g_1(C) \\ \vdots \\ g_m(C) \end{pmatrix},$$

i.e.,

$$g(C) = \begin{pmatrix} ((f(\langle u_0 \rangle + \sum_{j=1}^m (1 + \varepsilon \lambda_j) c_{j,m} w_j), w_1)) \\ \vdots \\ ((f(\langle u_0 \rangle + \sum_{j=1}^m (1 + \varepsilon \lambda_j) c_{j,m} w_j), w_m)) \end{pmatrix}.$$

In particular, we can rewrite (4.29)-(4.30) in the form

$$(4.31) \quad C' = G(C),$$

$$(4.32) \quad C(0) = C_0,$$

where

$$G(C) = - \begin{pmatrix} \frac{\lambda_1}{1+\varepsilon\lambda_1}g_1(C) + \frac{\lambda_1^2}{1+\varepsilon\lambda_1} \\ \cdot \\ \cdot \\ \cdot \\ \frac{\lambda_m}{1+\varepsilon\lambda_m}g_1(C) + \frac{\lambda_m^2}{1+\varepsilon\lambda_m} \end{pmatrix}$$

and

$$C(0) = \begin{pmatrix} c_1(0) \\ \cdot \\ \cdot \\ \cdot \\ c_m(0) \end{pmatrix}.$$

We can easily prove that G is locally Lipschitz continuous, so that the Cauchy–Lipschitz theorem yields the existence and uniqueness of the maximal solution to (4.31)–(4.32).

It thus follows from the above that we actually have the existence and uniqueness of the maximal solution to

$$(4.33) \quad \frac{d}{dt}(((-\Delta)^{-1}\bar{u}_m, w)) + ((\nabla v_m, \nabla w)) + ((f(u_m), w)) = 0, \quad \forall w \in W_m,$$

$$(4.34) \quad \bar{u}_m = \bar{v}_m - \varepsilon \Delta \bar{u}_m,$$

$$(4.35) \quad \bar{u}_m|_{t=0} = \bar{u}_{0,m},$$

where

$$(4.36) \quad u_m = \langle u_0 \rangle + \bar{u}_m, \quad v_m = \langle u_0 \rangle + \bar{v}_m.$$

We can now repeat the a priori estimates performed in the previous section, which are now fully justified at the approximated level, and pass to the limit. Here, the passage to the limit, as well as the continuity on u and v , is standard. In particular, as far as the nonlinear term $f(u_m)$ is concerned, we can note that it follows from standard Aubin–Lions compactness results that, at least for a subsequence that we do not relabel,

$$u_m \rightarrow u \text{ in } L^4(\Omega \times (0, T)) \text{ weakly and a.e.,}$$

for a proper u , which implies that

$f(u_m) \rightarrow f(u)$ a.e. and $f(u_m)$ is bounded in $L^{\frac{4}{3}}(\Omega \times (0, T))$.

Therefore, $f(u_m) \rightarrow f(u)$ in $L^{\frac{4}{3}}(\Omega \times (0, T))$ weakly (see, e.g., [6]), which is sufficient to pass to the limit in the weak formulation. Furthermore, since, e.g.,

$$u \in L^2(0, T; H^1(\Omega)) \text{ and } \frac{\partial u}{\partial t} \in L^2(0, T; H^1(\Omega)'),$$

then $u \in \mathcal{C}([0, T]; L^2(\Omega))$ and the weak continuity follows from the Strauss lemma (see, e.g., [14]).

□

5. CONVERGENCE TO THE CAHN–HILLIARD EQUATION

We call $(u^\varepsilon, v^\varepsilon)$ the solution to (4.1)–(4.5), as given in Theorem 4.1. Note that $(u^\varepsilon, v^\varepsilon)$ solves, for $T > 0$ given,

$$(5.1) \quad \frac{d}{dt}(((-\Delta)^{-1} \bar{u}^\varepsilon, w)) + ((\nabla v^\varepsilon, \nabla w)) + ((f(u^\varepsilon), w)) = 0 \text{ in } L^1(0, T), \forall w \in \bar{H}^1(\Omega),$$

$$(5.2) \quad u^\varepsilon = v^\varepsilon - \varepsilon \Delta v^\varepsilon \text{ in } L^2(0, T; H^1(\Omega)),$$

$$(5.3) \quad \langle u^\varepsilon \rangle = \langle u_0 \rangle, \quad t \geq 0, \text{ in } L^2(0, T),$$

$$(5.4) \quad u^\varepsilon|_{t=0} = u_0 \text{ in } L^4(\Omega)_{\mathbf{w}}.$$

It follows from the uniform (with respect to ε) a priori estimates derived in Section 3 and standard Aubin–Lions compactness results that, at least for a subsequence that we do not relabel, there exist (u^0, v^0) and φ such that, in particular,

$$u^\varepsilon \rightarrow u^0 \text{ in } L^\infty(0, T; L^4(\Omega)) \text{ weak star, in } L^2(0, T; H^1(\Omega)) \text{ weakly and a.e.,}$$

$$\frac{\partial u^\varepsilon}{\partial t} \rightarrow \frac{\partial u^0}{\partial t} \text{ in } L^2(0, T; H^1(\Omega)') \text{ weakly,}$$

$$v^\varepsilon \rightarrow v^0 \text{ in } L^\infty(0, T; H^1(\Omega)) \text{ weak star and } L^2(0, T; H^2(\Omega)) \text{ weakly}$$

and

$$\varepsilon^{\frac{1}{2}} v^\varepsilon \rightarrow \varphi \text{ in } L^\infty(0, T; H^2(\Omega)) \text{ weak star and } L^2(0, T; H^3(\Omega)) \text{ weakly.}$$

Actually, writing

$$u^\varepsilon = v^\varepsilon + \varepsilon^{\frac{1}{2}}(-\varepsilon^{\frac{1}{2}} \Delta v^\varepsilon),$$

we can see that

$$v^0 = u^0.$$

Having this, it is now standard to pass to the limit in (5.2)-(5.4) to find, at the limit,

$$(5.5) \quad \frac{d}{dt}(((-\Delta)^{-1} \bar{u}^0, w)) + ((\nabla u^0, \nabla w)) + ((f(u^0), w)) = 0 \text{ in } L^1(0, T), \quad \forall w \in \bar{H}^1(\Omega),$$

$$(5.6) \quad \langle u^0 \rangle = \langle u_0 \rangle, \quad t \geq 0, \text{ in } L^2(0, T),$$

$$(5.7) \quad u^0|_{t=0} = u_0 \text{ in } L^4(\Omega)_w,$$

i.e., u^0 is solution to the original Cahn–Hilliard equation. In particular, the convergence of the nonlinear term $f(u^\varepsilon)$ is similar to what was done in the previous section.

Noting finally that the solution to the Cahn–Hilliard equation is unique, we see that the whole sequence $(u^\varepsilon, v^\varepsilon)$ converges.

We have thus proved the following.

Theorem 5.1. *Under the assumptions of Theorem 4.1, the solution $(u^\varepsilon, v^\varepsilon)$ to (4.33)-(4.35) converges in $L^\infty(0, T; L^4(\Omega))$ weak star (for u^ε) and $L^2(0, T; H^1(\Omega))$ weakly (for v^ε) to the solution u^0 to the original Cahn–Hilliard equation, $\forall T > 0$.*

We also have the following.

Theorem 5.2. *We assume that the assumptions of Theorem 4.1 hold. Let $(u^\varepsilon, v^\varepsilon)$ and u^0 be the solutions to (4.1)-(4.5) and to the original Cahn–Hilliard equation, respectively, with the same initial datum u_0 . Then, $\forall T > 0$,*

$$\|u^\varepsilon - u^0\|_{L^\infty(0, T; H^1(\Omega)')} \leq c_T \varepsilon^{\frac{1}{2}},$$

$$\|v^\varepsilon - v^0\|_{L^2(0, T; H^1(\Omega))} \leq c_T \varepsilon^{\frac{1}{2}},$$

where c_T is independent of ε .

Proof. We can rewrite the Cahn–Hilliard equation in the following equivalent form:

$$(5.8) \quad (-\Delta)^{-1} \frac{\partial u^0}{\partial t} - \Delta v^0 + \overline{f(u^0)} = 0,$$

$$(5.9) \quad u^0 = v^0,$$

$$(5.10) \quad \langle u^0 \rangle = \langle u_0 \rangle, \quad t \geq 0,$$

$$(5.11) \quad \frac{\partial u^0}{\partial \nu} = 0 \text{ on } \Gamma,$$

$$(5.12) \quad u^0|_{t=0} = u_0.$$

Next, set $(u, v) = (u^\varepsilon, v^\varepsilon) - (u^0, v^0)$. Note that

$$(5.13) \quad \langle u \rangle = \langle v \rangle = 0, \quad t \geq 0.$$

Furthermore, (u, v) solves

$$(5.14) \quad (-\Delta)^{-1} \frac{\partial u}{\partial t} - \Delta v + \overline{f(u^\varepsilon) - f(u^0)} = 0,$$

$$(5.15) \quad u = v - \varepsilon \Delta v^\varepsilon,$$

$$(5.16) \quad \frac{\partial v}{\partial \nu} = 0 \text{ on } \Gamma,$$

$$(5.17) \quad u|_{t=0} = 0.$$

Multiplying (5.14) by u , we obtain, noting once more that $f' \geq -1$,

$$(5.18) \quad \frac{1}{2} \frac{d}{dt} \|u\|_{-1}^2 - ((u, \Delta v)) \leq \|u\|^2.$$

Note that, employing the interpolation inequality

$$\|u\|^2 \leq \|u\|_{-1} \|\nabla u\|,$$

we can write, owing to (5.15),

$$(5.19) \quad \|u\|^2 \leq \|u\|_{-1} \|\nabla v\| + \varepsilon \|u\|_{-1} \|\nabla \Delta v^\varepsilon\|.$$

Moreover, employing again (5.15), we can see that

$$(5.20) \quad -((u, \Delta v)) = \|\nabla v\|^2 - \varepsilon((\nabla v, \nabla \Delta v^\varepsilon)).$$

It thus follows from (5.18)-(5.20) that

$$\frac{1}{2} \frac{d}{dt} \|u\|_{-1}^2 + \|\nabla v\|^2 \leq \|u\|_{-1} \|\nabla v\| + \varepsilon \|u\|_{-1} \|\nabla \Delta v^\varepsilon\| + \varepsilon \|\nabla v\| \|\nabla \Delta v^\varepsilon\|,$$

which yields, employing Young's inequality,

$$(5.21) \quad \frac{d}{dt} \|u\|_{-1}^2 + \|\nabla v\|^2 \leq c(\|u\|_{-1}^2 + \varepsilon^2 \|\nabla \Delta v^\varepsilon\|^2).$$

Applying Gronwall's lemma to (5.21) leads to

$$\|u\|_{-1}^2 \leq c_T \varepsilon^2 \int_0^T \|\nabla \Delta v^\varepsilon\|^2 ds, \quad t \in [0, T], \quad T > 0 \text{ given,}$$

so that, recalling that $\varepsilon^{\frac{1}{2}} \|\nabla \Delta v^\varepsilon\|$ is bounded, independently of ε , in $L^2(0, T)$,

$$\|u(t)\|_{-1} \leq c_T \varepsilon^{\frac{1}{2}},$$

where c_T is independent of ε . Integrating next (5.21) over $(0, T)$, we find, similarly,

$$\int_0^T \|\nabla v\|^2 ds \leq c_T \varepsilon,$$

where c_T is independent of ε , which finishes the proof. □

Remark 5.3. We can obtain a similar result if we take

$$u^\varepsilon|_{t=0} = u_\varepsilon^0, \quad u^0|_{t=0} = u_0,$$

where

$$\|u_\varepsilon^0 - u_0\|_{-1} \leq \varepsilon^{\frac{1}{2}}.$$

6. THE CASE OF LOGARITHMIC NONLINEAR TERMS

We now take

$$f(s) = -c_0 s + c_1 \ln\left(\frac{1+s}{1-s}\right), \quad s \in (-1, 1), \quad 0 < c_1 < c_0.$$

Note that the condition $c_1 < c_0$ is made to ensure that the potential

$$\begin{aligned} F(s) &= \int_0^s f(\xi) d\xi \\ &= -\frac{c_0}{2} s^2 + c_1((1+s) \ln(1+s) + (1-s) \ln(1-s)) \end{aligned}$$

has a double-well structure. These functions satisfy

$$(6.1) \quad f' \geq -c_0, \quad F \geq -c_2, \quad c_2 \geq 0,$$

$$(6.2) \quad f(s)(s-m) \geq c_3(m)(|f(s)| + F(s)) - c_4(m), \quad s, m \in (-1, 1),$$

where $c_3(m) > 0$ and $c_4(m) \geq 0$ depend continuously on m (see, e.g., [10]).

Remark 6.1. Such a logarithmic potential was already proposed in [2] and is the thermodynamically relevant one. In particular, the logarithmic terms correspond to the entropy of mixing.

We then consider, for $N \in \mathbb{N}$, $N \geq 2$, the \mathcal{C}^1 -functions defined on the real line by

$$f_N(s) = \begin{cases} f(1 - \frac{1}{N}) + f'(1 - \frac{1}{N})(s - 1 + \frac{1}{N}), & s > 1 - \frac{1}{N}, \\ f(s), & s \in [-1 + \frac{1}{N}, 1 - \frac{1}{N}], \\ f(-1 + \frac{1}{N}) + f'(-1 + \frac{1}{N})(s + 1 - \frac{1}{N}), & s < -1 + \frac{1}{N}. \end{cases}$$

In particular,

$$(6.3) \quad f'_N \geq -c_0, \quad F_N \geq -c_5, \quad c_5 \geq 0,$$

and, for N large enough,

$$(6.4) \quad f_N(s)(s - m) \geq c_6(m)(|f_N(s)| + F_N(s)) - c_7(m), \quad s \in \mathbb{R}, \quad m \in (-1, 1),$$

where $c_6(m) > 0$ and $c_7(m) \geq 0$ are independent of N and $F_N(s) = \int_0^s f_N(\xi) d\xi$; here, the constants $c_6(m)$ and $c_7(m)$ depend continuously on m .

We next introduce the approximated problems

$$(6.5) \quad \frac{\partial u_N}{\partial t} + \Delta^2 v_N - \Delta f_N(u_N) = 0,$$

$$(6.6) \quad u_N = v_N - \varepsilon \Delta v_N,$$

$$(6.7) \quad \frac{\partial u_N}{\partial \nu} = \frac{\partial v_N}{\partial \nu} = \frac{\partial \Delta v_N}{\partial \nu} = 0 \text{ on } \Gamma,$$

$$(6.8) \quad u_N|_{t=0} = u_0.$$

The existence and uniqueness of the solution to (6.5)-(6.8) can be proved as in Section 2, noting that f_N has a linear growth at infinity and is of class \mathcal{C}^1 .

We can also perform the same a priori estimates as in Section 2. In particular, we have

$$(6.9) \quad \frac{d}{dt}(\|\nabla v_N\|^2 + \varepsilon \|\Delta v_N\|^2 + 2 \int_{\Omega} F_N(u_N) dx) + 2 \left\| \frac{\partial u_N}{\partial t} \right\|_{-1}^2 = 0,$$

$$(6.10) \quad \frac{d}{dt}(\varepsilon \|u_N\|^2) + (1 - \varepsilon_0) \|\nabla u_N\|^2 \leq \frac{1}{1 - \varepsilon_0} \|\nabla v_N\|^2$$

and

$$(6.11) \quad \frac{d}{dt} \|u_N\|^2 + \|\Delta v_N\|^2 + \varepsilon \|\nabla \Delta v_N\|^2 \leq 2 \|\nabla u_N\|^2.$$

Next, it follows from (6.5) that

$$\overline{f_N(u_N)} = -(-\Delta)^{-1} \frac{\partial u_N}{\partial t} + \Delta v_N,$$

which yields, in view of the above estimates, that $\overline{f_N(u_N)} \in L^2(\Omega \times (0, T))$, $T > 0$ given. Furthermore, we can write

$$|\langle f_N(u_N) \rangle| \leq c \int_{\Omega} |f_N(u_N)| dx$$

and it follows from (6.2), taking $s = u_N$ and $m = \langle u_N \rangle (= \langle u_0 \rangle)$, that

$$\begin{aligned} |\langle f_N(u_N) \rangle| &\leq c((f_N(u_N), \bar{u}_N)) + c' \\ &= c(\overline{(f_N(u_N), u_N)}) + c' \leq c \|\overline{f_N(u_N)}\| \|u_N\| + c', \end{aligned}$$

which yields that $\langle f_N(u_N) \rangle \in L^2(0, T)$, so that, finally, we recover the full L^2 -norm and deduce that $f_N(u_N) \in L^2(\Omega \times (0, T))$.

These estimates allow to pass to the limit $N \rightarrow +\infty$ in the equations, following [10]. Here, again, the only difficulty is to pass to the limit in the nonlinear term $f_N(u_N)$. First, it follows from the above that $f_N(u_N)$ is bounded, independently of N , in $L^1(\Omega \times (0, T))$. Then, it follows from the explicit expression of f_N that, for N large enough,

$$(6.12) \quad \text{meas}(E_{N,M}) \leq \varphi\left(\frac{1}{N}\right), \quad N \leq M,$$

where

$$E_{N,M} = \{(x, t) \in \Omega \times (0, T), |u_M(x, t)| > 1 - \frac{1}{N}\}$$

and

$$\varphi(s) = \frac{c}{|f(1-s)|}, \quad s \in (0, 1).$$

Note indeed that, taking N (and, thus, M) large enough (also note that f and f_N are odd),

$$\begin{aligned}
c &\geq \int_0^T \int_{\Omega} |f_M(u_M)| \, dx \, dt \geq \int_{E_{N,M}} |f_M(u_M)| \, dx \, dt \\
&\geq \text{meas}(E_{N,M}) f(1 - \frac{1}{N}).
\end{aligned}$$

We can now pass to the limit $M \rightarrow +\infty$ (employing Fatou's lemma) and then $N \rightarrow +\infty$ (noting that $\lim_{s \rightarrow 0} \varphi(s) = 0$) in (6.12) to find

$$\text{meas}\{(x, t) \in \Omega \times (0, T), \, |u(x, t)| \geq 1\} = 0,$$

so that

$$(6.13) \quad -1 < u(x, t) < 1 \text{ for a.a. } (x, t) \in \Omega \times (0, T).$$

Next, it follows from the almost everywhere convergence of u_N to u (that again follows from standard Aubin–Lions compactness results and holds at least for a subsequence that we do not relabel), (6.13) and the explicit expression of f_N that

$$(6.14) \quad f_N(u_N(x, t)) \rightarrow f(u(x, t)) \text{ for a.a. } (x, t) \in \Omega \times (0, T).$$

Finally, since $f_N(u_N)$ is bounded, independently of N , in $L^2(\Omega \times (0, T))$, it follows from (6.14) that $f_N(u_N) \rightarrow f(u)$ in $L^2(\Omega \times (0, T))$ weakly, which allows to pass to the limit in the variational formulation.

We thus have the following.

Theorem 6.2. *We assume that (2.5) holds and that $u_0 \in H^1(\Omega)$ and $\varepsilon u_0 \in H^2(\Omega)$, with $-1 < u_0(x) < 1$ for a.a. $x \in \Omega$. Then (6.5)–(6.8) possesses a unique weak solution (u, v) such that, $\forall T > 0$,*

$$u \in L^\infty(\mathbb{R}^+; L^2(\Omega)) \cap L^2(0, T; H^1(\Omega)),$$

$$\frac{\partial u}{\partial t} \in L^2(\mathbb{R}^+; H^1(\Omega)'),$$

$$v \in L^\infty(\mathbb{R}^+; H^2(\Omega)) \cap L^2(0, T; H^3(\Omega)),$$

$$\frac{\partial v}{\partial t} \in L^2(\mathbb{R}^+; H^1(\Omega)).$$

Furthermore, $u \in \mathcal{C}([0, T]; L^2(\Omega))$, $v \in C([0, T]; H^2(\Omega))$ and

$$-1 < u(x, t) < 1 \text{ for a.a. } (x, t) \in \Omega \times (0, T).$$

One open problem is now to pass to the limit as $\varepsilon \rightarrow 0$. More precisely, we can pass to the limit and see that the solution to (6.5)-(6.8) converges to the solution u^0 to a problem of the form (we consider here a weak form of the equations)

$$(6.15) \quad (-\Delta)^{-1} \frac{\partial u^0}{\partial t} - \Delta v^0 + \xi = 0,$$

$$(6.16) \quad u^0 = v^0,$$

$$(6.17) \quad \langle u^0 \rangle = \langle u_0 \rangle, \quad t \geq 0,$$

$$(6.18) \quad \frac{\partial u^0}{\partial \nu} = 0 \text{ on } \Gamma,$$

$$(6.19) \quad u^0|_{t=0} = u_0.$$

The difficulty is then to prove that $\xi = \overline{f(u^0)}$. Recall that to prove that $f_N(u_N)$ converges to $f(u)$, one uses the explicit form of the approximated functions f_N . This argument can no longer be employed to study the convergence of $f(u^\varepsilon)$ and prove that, at the limit,

$$-1 < u^0(x, t) < 1 \text{ for a.a. } (x, t) \in \Omega \times (0, T), \quad T > 0.$$

Remark 6.3. Writing $(u^{N,\varepsilon}, v^{N,\varepsilon})$ the solution to (6.5)-(6.8), we can prove, proceeding as in the previous section (recall that f_N has a linear growth at infinity), that $(u^{N,\varepsilon}, v, N^\varepsilon)$ converges to (u^N, v^N) as $N \rightarrow +\infty$, where (u^N, v^N) is solution to the Cahn–Hilliard system

$$(6.20) \quad (-\Delta)^{-1} \frac{\partial u^N}{\partial t} - \Delta v^N + \overline{f_N(u^N)} = 0,$$

$$(6.21) \quad u^N = v^N,$$

$$(6.22) \quad \langle u^N \rangle = \langle u_0 \rangle, \quad t \geq 0,$$

$$(6.23) \quad \frac{\partial u^N}{\partial \nu} = 0 \text{ on } \Gamma,$$

$$(6.24) \quad u^N|_{t=0} = u_0.$$

We can then pass to the limit $N \rightarrow \infty$ and deduce (following [10]) that (u^N, v^N) converges to the solution (u^0, v^0) to the Cahn–Hilliard system with a logarithmic nonlinear term f ,

$$(6.25) \quad (-\Delta)^{-1} \frac{\partial u^0}{\partial t} - \Delta v^0 + \overline{f(u^0)} = 0,$$

$$(6.26) \quad u^0 = v^0,$$

$$(6.27) \quad \langle u^0 \rangle = \langle u_0 \rangle, \quad t \geq 0,$$

$$(6.28) \quad \frac{\partial u^0}{\partial \nu} = 0 \text{ on } \Gamma,$$

$$(6.29) \quad u^0|_{t=0} = u_0.$$

In that case, we have the separation property

$$-1 < u^0(x, t) < 1 \text{ for a.a. } (x, t) \in \Omega \times (0, T), \quad T > 0.$$

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