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On a nonlocal phase separation model

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Abstract

An alternative to the Cahn–Hilliard model of phase separation for two–phase systems in a simplified isothermal case is given. It introduces nonlocal terms and allows reasonable bounds for the concentrations. Using the free energy as Lyapunov functional the asymptotic state of the system is investigated and characterized by a variational principle.

1. Introduction

We consider a binary alloy with components A and B occupying a spatial domain Ω. We denote by u and $1-u$ the (scaled) local concentrations of A and B, respectively. Let $(0,T)$ denote a time interval, ν the outer unit normal on the (sufficiently smooth) boundary $\Gamma = \partial\Omega$, and $Q = (0,T) \times \Omega$, $\Gamma_T = (0,T) \times \Gamma$. To describe phase separation in binary systems one uses usually the Cahn–Hilliard equation. This equation is derived ([CH]) from a free energy functional of the form

$$F_{CH}(u) = \int_\Omega \left\{ f(u) + \kappa\, u\,(1-u) + \frac{\lambda}{2} \left|\nabla u\right|^2 \right\} dx. \tag{1.1}$$

Here f is a convex function with the property that $f(u) + \kappa u(1-u)$ (for sufficiently large κ) forms a so–called double well potential. Adapting classical thermodynamical relations one introduces a chemical potential v as gradient of the free energy:

$$v = f'(u) + \kappa\,(1-2u) - \lambda\Delta u. \tag{1.2}$$

Now one postulates that $-\nabla v$ is the driving force for the mass flux $\mathbf{j}$, i.e.,

$$\mathbf{j} = -\mu\nabla v$$

with a suitable mobility μ. Considering the mass balance one ends up with the Cahn–Hilliard equation

$$\frac{\partial u}{\partial t} - \nabla\cdot(\,\mu\,(f'(u) + \kappa\,(1-2u) - \lambda\Delta u)) = 0 \;\text{ in } Q, \quad \nu\cdot(\mu\nabla v) = 0 \;\text{ on } \Gamma_T, \tag{1.3}$$

where the boundary condition guarantees mass conservation

$$\int_\Omega u(t,x)dx = \int_\Omega u(0,x)dx.$$

Inspecting Cahn–Hilliard's arguments ([CH]) establishing (1.1) as the free energy of the binary system it seems to be reasonable and even more adequate ([GL1]) to choose an alternative expression like

$$F(u) = \int_\Omega \Big\{ f(u) + u \int_\Omega \mathcal{K}(|x-y|)(1-u(y))\,dy \Big\} dx, \tag{1.4}$$

where the kernel $\mathcal{K}$ of the integral term describes nonlocal interaction ([ChF]). This expression may be written in a form more similar to (1.1):

$$F(u) = \int_\Omega \Big\{ f(u) + \kappa_1 u(1-u) + \frac{1}{2}\int_\Omega \mathcal{K}(|x-y|)|u(x)-u(y)|^2\,dy \Big\} dx,$$

where

$$\kappa_1 = \kappa_1(x) = \int_\Omega \mathcal{K}(|x-y|)dy.$$

By a simple calculation we find from (1.4) the corresponding chemical potential v as the gradient of F in the form

$$v = f'(u) + w, \quad w(x) = \int_\Omega \mathcal{K}(|x-y|)(1-2\,u(y))\,dy. \tag{1.5}$$

Replacing (1.2) by (1.5) one gets instead of (1.3) the equation

$$\frac{\partial u}{\partial t} - \nabla\cdot(\,\mu\,\nabla(f'(u)+w)) = 0.$$

Assuming that f is strictly convex, the strictly monotone function f' has an inverse function f'^{-1} . With this function we obtain as alternative to (1.3) the system

$$\frac{\partial}{\partial t}(f'^{-1}(v-w)) - \nabla\cdot(\mu\nabla v) = 0 \ \text{ in } Q, \quad \nu\cdot(\mu\nabla v) = 0 \ \text{ on } \Gamma_T, \tag{1.6}$$

$$v = f'(u) + w, \quad w(x) = \int_\Omega \mathcal{K}(|x-y|)(1-2\,u(y))\,dy. \tag{1.7}$$

As a consequence of (1.7) the a priori estimate

$$u(x) \in \text{im}\,(f'^{-1}) \tag{1.8}$$

holds automatically. In the standard case

$$f(u) = u\log u + (1-u)\log(1-u)$$

we have

$$f'(u) = \log\left(\frac{u}{1-u}\right) \quad \text{and} \quad f'^{-1}(v-w) = \frac{1}{1+\exp(w-v)}.$$

The image of the Fermi function $1/(1+\exp(s))$ is the interval $[0,1]$, so that the nonlocal model automatically satisfies the physical requirement $0 \le u(x) \le 1$. This property cannot be guaranteed for solutions of the original Cahn–Hilliard equation since for fourth order equations no maximum principle is available ([AP]). Elliot and Garcke ([EGa]) have proved this property for special mobilities but they have no uniqueness result.

Moreover, by physical reasons it is desirable to admit mobilities μ depending on u and $|\nabla v|$. A natural choice seems to be ([EGa],[Ga])

$$\mu = \frac{a(|\nabla v|)}{f''(u)} \tag{1.9}$$

with a function a such that $s \mapsto a(s)s$ is monotone. We shall show that the operator $(u,v) \mapsto -\nabla \cdot (\mu \nabla v)$ with such a μ is monotone in an appropriate sense ([Gaj]) and that (1.6), (1.7) has a unique solution provided $1/f''$ is concave. With (1.9) the equation (1.6) can be rewritten as

$$\begin{aligned} \frac{\partial u}{\partial t} - \nabla \cdot a\left(\nabla u + \frac{\nabla w}{f''(u)}\right) &= 0 \text{ in } Q, \\ \nu \cdot \left[a\left(\nabla u + \frac{\nabla w}{f''(u)}\right)\right] &= 0 \text{ on } \Gamma_T. \end{aligned}$$

We are indebted to A. Bovier for the hint that similar equations with a nonlocal term are studied in the papers ([GL1],[GL2]), starting from a stochastic background. It seems worth mentioning that drift–diffusion equations of this form also model transport processes in semiconductor ([GG]) and chemotaxis ([GZ]) theory.

In Section 2 we formulate the problem and the assumptions. In Section 3 we show existence and uniqueness of solutions and state some regularity properties of the solutions. In Section 4 we consider the asymptotic behaviour for time going to infinity and characterize the asymptotic state by a variational principle. Section 5 establishes a link with the theory of chemotaxis.

2. Formulation of the problem, assumptions

Let be $\Omega \subset \mathbb{R}^n$ a bounded Lipschitzian domain with boundary $\Gamma = \partial\Omega$ and ν the outer unit normal on Γ. Denote by $L^p = L^p(\Omega)$, $H^{1,p} = H^{1,p}(\Omega)$ for $1 \le p \le \infty$ the usual function spaces on Ω, $H^1 = H^{1,2}(\Omega)$, $\|\cdot\|_2 = \|\cdot\|$ the norm in L^2 and by $(\cdot,\cdot)$ the pairing between H^1 and its dual $(H^1)^*$ ([A],[GGZ],[KJF]). For a time interval $(0,T)$, $T > 0$, and a Banach space X we denote by $L^p(0,T;X)$ the usual spaces of Bochner integrable functions with values in X. We set $\mathbb{R}^1_+ = (0,\infty)$ and , as already mentioned, $Q = (0,T) \times \Omega$, $\Gamma_T = (0,T) \times \Gamma$. "Generic" positive constants are denoted by C.

We consider the problem

$$v = f'(u) + w, \quad w(t,x) = \int_\Omega \mathcal{K}(|x-y|)(1 - 2\,u(t,y))\,dy, \quad (t,x) \in Q, \tag{2.1}$$

$$\frac{\partial u}{\partial t} - \nabla \cdot (\mu \nabla v)) = 0 \quad \text{in} \quad Q, \qquad \mu\, \nu \cdot \nabla v = 0 \quad \text{on } \Gamma_T, \tag{2.2}$$

$$u(0,x) = u_0(x), \qquad x \in \Omega. \tag{2.3}$$

We assume:

(i) $f(u) = u \log u + (1-u)\log(1-u)$,

(ii) the kernel $\mathcal{K} \in (\mathbb{R}^1_+ \mapsto \mathbb{R}^1)$ is such that

$$\int_\Omega \int_\Omega \Big|\mathcal{K}(|x-y|)\Big| dx\, dy = m_0 < \infty, \quad \sup_{x\in\Omega} \int_\Omega \Big|\mathcal{K}(|x-y|)\Big|\, dy = m_1 < \infty$$

and the potential operator P defined by

$$\varrho \mapsto P\varrho = \int_\Omega (\mathcal{K}(|x-y|)\varrho(y) dy$$

satisfies

$$\|P\varrho\|_{H^{1,p}} \le r_p \|\varrho\|_{L^p}, \quad 1 \le p \le \infty.$$

(iii) the mobility μ has the form

$$\mu = \frac{a(x, |\nabla v|)}{f''(u)},$$

where $a \in (\Omega \times \mathbb{R}^1_+ \mapsto \mathbb{R}^1_+)$ is measurable with respect to x for all $s \in \mathbb{R}^1_+$ and continuous with respect to s for a. a. $x \in \Omega$ and satisfies

$$\begin{aligned} (a(x,s_1)s_1 - a(x,s_2)s_2)(s_1 - s_2) \ &\ge\ \alpha_0 |s_1 - s_2|^2, \quad s_1, s_2 \in \mathbb{R}^1_+, \\ |a(x,s_1)s_1 - a(x,s_2)s_2| \ &\le\ \alpha_1 |s_1 - s_2|, \quad \alpha_0 > 0,\ \alpha_1 > 0. \end{aligned}$$

(iv) $u_0 \in L^\infty(\Omega), \quad 0 \le u_0(x) \le 1, \quad x \in \Omega,$

$$\int_\Omega u_0(x)\, dx = u_\alpha |\Omega|, \quad 0 < u_\alpha = \text{const.} < 1, \quad |\Omega| = \text{ meas } (\Omega).$$

We note some elementary properties of the function f :

f is strongly convex, more precisely,

$$f(u_1) + f(u_2) - 2f\left(\frac{u_1+u_2}{2}\right) \ge (u_1-u_2)^2, \quad u_1, u_2 \in (0,1), \tag{2.4}$$

$$f'(u) = \log\frac{u}{1-u}, \quad (f')^{-1}(s) = \frac{1}{1+\exp(-s)}, \quad \text{im } (f')^{-1} = [\,0,1] \tag{2.5}$$

and the function

$$\frac{1}{f''(u)} = u(1-u)$$

is strongly concave because of

$$\frac{2}{f''\left(\frac{u_1+u_2}{2}\right)} - \frac{1}{f''(u_1)} - \frac{1}{f''(u_2)} = \frac{1}{2}\,(u_1-u_2)^2. \tag{2.6}$$

Remark 2.1. For simplicity, we restrict ourselves in this paper to the function mentioned in (i). Our results could be carried over to other strongly convex functions f for which $\operatorname{im}(f')^{-1} = [0,1]$ and $1/f''$ is a strongly concave function.

Remark 2.2. Examples for kernels $\mathcal{K}$ satisfying (ii) are Newton potentials ([LL]):

$$\mathcal{K}(|x|) = \kappa_n |x|^{2-n}, \quad n \neq 2; \quad \mathcal{K}(|x|) = -\kappa_2 \log|x|, \quad n=2; \quad \kappa_n = \text{ const.} > 0$$

and usual mollifiers like

$$\mathcal{K}(|x|) = \begin{cases} C\exp\left(-\dfrac{h^2}{h^2-|x|^2}\right) & \text{if } |x|<h, \\ 0 & \text{if } |x|\geq h, \end{cases}$$

where $h>0$ characterizes the range of the interaction.

Remark 2.3. Mobilities of the form

$$\mu = \frac{a}{f''(u)},$$

seem to be natural and were considered e.g. in [EGa], [GL1], [GL2], where $a=a(u)$.

Using (2.5) the system (2.1)–(2.3) can be reformulated as

$$w(t,x) = \int_\Omega \mathcal{K}(|x-y|)(1-2\,u(t,y))\,dy, \quad (t,x)\in Q, \tag{2.7}$$

$$u_t - \nabla\cdot(\,\mu\nabla v)) = 0 \ \text{ in } \ Q, \quad \mu\,\nu\cdot\nabla v = 0 \ \text{ on } \Gamma_T, \tag{2.8}$$

$$u = \frac{1}{1+\exp(w-v)}\,, \quad u(0,x)=u_0(x), \quad 0\leq u_0(x)\leq 1, \quad x\in\Omega. \tag{2.9}$$

Definition 2.1.
A triple (u,v,w) is called a solution of (2.7)–(2.9) if $u\in C(0,T;L^\infty)\cap L^2(0,T;H^1)$ with $u_t\in L^2(0,T;(H^1)^*)$ and $w\in C(0,T;H^{1,\infty})$ satisfy (2.7) and $v=f'(u)+w$ satisfies

$$\int_0^T\int_\Omega \mu|\nabla v|^2 dxdt < \infty$$

and

$$\int_0^T \left\{(u_t,h) + \int_\Omega \mu\nabla v\cdot\nabla h\,dx\right\} dt = 0, \quad \forall h\in L^2(0,T;H^1).$$

Note that the last identity for $h=1$ gives

$$\int_\Omega u(t,x)dx = \int_\Omega u_0(x)dx = u_\alpha|\Omega|. \tag{2.10}$$

3. Existence, uniqueness, regularity

First of all we want to prove a priori estimates. Here a key rôle plays the free energy given by (1.4).

Lemma 3.1. *Let* (u,v,w) *be a solution of* (2.6)–(2.8). *Then*

$$\frac{d}{dt}F(u(t)) \le -\alpha_0 \int_\Omega \frac{|\nabla v|^2}{f''(u)}\,dx \le 0, \tag{3.1}$$

$$\int_0^T \int_\Omega \frac{|\nabla v|^2}{f''(u)}\,dx \le C < \infty, \tag{3.2}$$

where C *is a constant which not depends on* T .

Proof. The estimate (3.1) follows from

$$\begin{aligned}\frac{d}{dt}F(u(t)) &= (u_t, f'(u)+w) = -\int_\Omega \mu\,|\nabla v|^2\,dx \\ &= -\int_\Omega \frac{a}{f''(u)}|\nabla v|^2 dx \le -\alpha_0 \int_\Omega \frac{|\nabla v|^2}{f''(u)}\,dx.\end{aligned}$$

Using $0 \le u(x) \le 1$, $u\log u \ge -1/e$ and the properties of the kernel $\mathcal{K}$, we find

$$\begin{aligned}F(u(t)) &= \int_\Omega \Big\{u\log u + (1-u)\log(1-u) + u\int_\Omega \mathcal{K}(|x-y|)(1-u(y))dy\Big\}dx \\ &\ge -\frac{2|\Omega|}{e} - m_0.\end{aligned}$$

Hence (3.1) implies

$$\begin{aligned}\int_0^T \int_\Omega \frac{|\nabla v|^2}{f''(u)}\,dx &\le -\frac{1}{\alpha_0}\int_0^T \frac{d}{dt}F(u(t))\,dt = \frac{1}{\alpha_0}\left[F(u_0) - F(u(t))\right] \\ &\le \frac{1}{\alpha_0}\left[F(u_0) + \frac{2|\Omega|}{e} + m_0\right] = C,\end{aligned}$$

where C is independent of T . □

We define by

$$
\begin{aligned}
(A(v,w),h) &= \int_\Omega \mu(v,w)\nabla v\cdot\nabla h dx, \quad \forall h\in H^1,\\
\mu(v,w) &= \frac{a(|\nabla v|)}{f''(u)}, \quad u=\frac{1}{1+\exp(w-v)},
\end{aligned}
$$

an operator $A\in(D(A)\mapsto(H^1)^*)$, where

$$
D(A)=\{(v,w):\int_\Omega \mu(v,w)|\nabla v|^2<\infty,\ w\in H^1\}.
$$

The following monotonicity property of A is the main tool for proving uniqueness results.

Lemma 3.2. *Let*

$$
(v_i,w_i)\in D(A),\quad u_i=\frac{1}{1+\exp(z_i)},\quad z_i=w_i-v_i,\ (i=1,2),\quad u_m=\frac{u_1+u_2}{2}.
$$

Then

$$
\begin{aligned}
\delta &= (A(v_1,w_1),f'(u_1)-f'(u_m))+(A(v_2,w_2),f'(u_2)-f'(u_m))\\
&\geq -\frac{\alpha_1}{4}\left(r_\infty^2\|u_1-u_2\|^2+\frac{\alpha_1}{8\alpha_0}\Big\|\nabla(w_1-w_2)\Big\|^2\right).
\end{aligned}
$$

Proof. Set $f_i'=f'(u_i)$, $f_i''=f''(u_i)$, $\mu_i=\mu(v_i,w_i)$, $a_i=a(|\nabla v_i|)$, $(i=1,2,m)$. We have

$$
\begin{aligned}
\delta &= \int_\Omega\{\mu_1\nabla v_1\cdot\nabla(f_1'-f_m')+\mu_2\nabla v_2\cdot\nabla(f_2'-f_m')\}dx\\
&= \int_\Omega\left\{\mu_1\nabla v_1\cdot\left[\nabla z_1-\frac{f_m''}{2}\left(\frac{\nabla z_1}{f_1''}+\frac{\nabla z_2}{f_2''}\right)\right]\right.\\
&\qquad\left.+\mu_2\nabla v_2\cdot\left[\nabla z_2-\frac{f_m''}{2}\left(\frac{\nabla z_1}{f_1''}+\frac{\nabla z_2}{f_2''}\right)\right]\right\}dx\\
&= \int_\Omega\frac{f_m''}{2}\left\{\left(\frac{2}{f_m''}-\frac{1}{f_1''}-\frac{1}{f_2''}\right)\left(\frac{a_1\nabla v_1\cdot\nabla z_1}{f_1''}+\frac{a_2\nabla v_2\cdot\nabla z_2}{f_2''}\right)\right.\\
&\qquad\left.+\frac{1}{f_1''f_2''}(a_1\nabla v_1-a_2\nabla v_2)\cdot\nabla(z_1-z_2)\right\}dx.
\end{aligned}
$$

Now, using the concavity of $1/f''$ (see (2.6)), the assumptions (i)–(iii) and $1/f''(u)=u(1-u)$, we get

$$
\delta \geq -\int_\Omega\frac{f_m''}{2}\left\{\frac{\alpha_1}{8}(u_1-u_2)^2\left[\frac{|\nabla w_1|^2}{f_1''}+\frac{|\nabla w_2|^2}{f_2''}\right]\right.
$$

$$+\frac{\alpha_1^2}{4\alpha_0 f_1'' f_2''}|\nabla(w_1-w_2)|^2\Big\}dx$$

$$\geq \quad -\frac{\alpha_1}{8}\int_\Omega\Big\{(u_1-u_2)^2(|\nabla w_1|^2+|\nabla w_2|^2)+\frac{\alpha_1}{4\alpha_0}|\nabla(w_1-w_2)|^2\Big\}dx$$

$$\geq \quad -\frac{\alpha_1}{4}\left(r_\infty^2\|u_1-u_2\|^2+\frac{\alpha_1}{8\alpha_0}\Big\|\nabla(w_1-w_2)\Big\|^2\right).$$

This is our assertion. □

Lemma 3.3. *Let* $w\in L^\infty(0,T;H^{1,\infty})$ *be given. Then the problem*

$$u_t+A(v,w)=0,\quad u=\frac{1}{1+\exp(w-v)},\quad u(0)=u_0, \tag{3.3}$$

has a unique solution $v=v(w)$ *such that*

$$\int_0^T\int_\Omega\mu(v,w)|\nabla v|^2dxdt<\infty. \tag{3.4}$$

Proof. **Existence.**
We consider the regularized problem

$$u_t+A_\varepsilon(v,w)=0,\quad u=\frac{1}{1+\exp(w-v)},\quad u(0)=u_0, \tag{3.5}$$

with

$$(A_\varepsilon(v,w),h)=\int_\Omega\mu_\varepsilon(v,w)\nabla v\cdot\nabla h dx,\quad \forall h\in H^1,\quad \mu_\varepsilon=\mu+\varepsilon\ \ (\varepsilon>0).$$

By results of ([ALu]) there exists a solution $v_\varepsilon\in L^2(0,T;H^1)$ with $u_{\varepsilon t}\in L^2(0,T;(H^1)^*)$. We consider the functional

$$F_w(u)=\int_\Omega f(u)\,dx+\int_0^T(u_t,w)\,ds.$$

We have

$$\frac{d}{dt}F_w(u)=(u_t,w)+\int_\Omega f'(u)\,u_t\,dx=(u_t,w+f'(u))$$

and by arguments similar to those used in the proof of Lemma 3.1 we can show that

$$\frac{d}{dt}F_w(u_\varepsilon)=\leq -\alpha_0\int_\Omega\frac{|\nabla v_\varepsilon|^2}{f''(u_\varepsilon)}dx\ \leq\ 0,$$

i.e., F_w is a Lyapunov functional for (3.5) – a functional decaying in time along a solution u_ε. From

$$\frac{d}{dt}F_w(u_\varepsilon)=-\int_\Omega\mu_\varepsilon|\nabla v_\varepsilon|^2dx$$

follows by integration

$$
\begin{aligned}
\int_0^T \int_\Omega \mu_\varepsilon |\nabla v_\varepsilon|^2 dxdt &= -\int_0^T \frac{d}{dt} F_w(u_\varepsilon) dt = -\int_0^T (u_{\varepsilon t}, f'(u_\varepsilon) + w) dt \\
&= -\int_0^T \frac{d}{dt} f(u_\varepsilon) dt - \int_0^T (u_{\varepsilon t}, w) dt \\
&= f(u(0)) - f(u_\varepsilon(T)) - \int_0^T (u_{\varepsilon t}, w) dt \\
&\leq |f(u(0))| + \frac{2|\Omega|}{e} + \int_0^T \|u_{\varepsilon t}\|_{(H^1)^*} \|w\|_{H^1} dt \\
&\leq C + \|u_{\varepsilon t}\|_{L^2(0,T;(H^1)^*)} \|w\|_{L^2(0,T;H^1)} .
\end{aligned}
$$

On the other hand, we have

$$
\begin{aligned}
\|u_{\varepsilon t}\|_{L^2(0,T;(H^1)^*)} &= \sup_{h \in L^2(0,T;H^1)} \frac{\left| \int_0^T (u_{\varepsilon t}, h) dt \right|}{\|h\|_{L^2(0,T;H^1)}} \\
&= \sup_{h \in L^2(0,T;H^1)} \frac{\left| \int_0^T \int_\Omega \mu_\varepsilon \nabla v_\varepsilon \cdot \nabla h \, dx \, dt \right|}{\|h\|_{L^2(0,T;H^1)}} \\
&\leq \left(\int_0^T \int_\Omega \mu_\varepsilon^2 |\nabla v_\varepsilon|^2 dx \, dt \right)^{1/2} .
\end{aligned}
$$

We take into account $0 \leq u_\varepsilon \leq 1$, choose $0 < \varepsilon \leq 1$ and get

$$
\mu_\varepsilon \;=\; \varepsilon + \frac{a(|\nabla v_\varepsilon|}{f''(u_\varepsilon)} \;\leq\; \varepsilon + \alpha_1 u_\varepsilon (1 - u_\varepsilon) \;\leq\; 1 + \frac{\alpha_1}{4},
$$

hence

$$
\|u_{\varepsilon t}\|_{L^2(0,T;(H^1)^*)} \leq \sqrt{1 + \frac{\alpha_1}{4}} \left(\int_0^T \int_\Omega \mu_\varepsilon |\nabla v_\varepsilon|^2 dx \, dt \right)^{1/2} .
$$

So the estimate above becomes

$$
\int_0^T \int_\Omega \mu_\varepsilon |\nabla v_\varepsilon|^2 dxdt \leq C + \|w\|_{L^2(0,T;H^1)} \sqrt{1 + \frac{\alpha_1}{4}} \left(\int_0^T \int_\Omega \mu_\varepsilon |\nabla v_\varepsilon|^2 dx \, dt \right)^{1/2} .
$$

By the usual argumentation we obtain

$$
\int_0^T \int_\Omega \mu_\varepsilon |\nabla v_\varepsilon|^2 dxdt \leq C < \infty \quad \text{and} \quad \|u_{\varepsilon t}\|_{L^2(0,T;(H^1)^*)} \leq C < \infty \quad (0 < \varepsilon \leq 1). \tag{3.6}
$$

On the other hand, the estimate

$$\begin{aligned}\int_\Omega \mu_\varepsilon |\nabla v_\varepsilon|^2 dx &\geq \alpha_0 \int_\Omega \frac{|\nabla v_\varepsilon|^2}{f''(u_\varepsilon)}\, dx = \alpha_0 \int_\Omega \frac{|f''(u_\varepsilon)\nabla u_\varepsilon + \nabla w|^2}{f''(u_\varepsilon)}\, dx \\ &= \alpha_0 \int_\Omega \left(f''(u_\varepsilon)|\nabla u_\varepsilon|^2 + 2\,\nabla u_\varepsilon \cdot \nabla w + \frac{|\nabla w|^2}{f''(u_\varepsilon)} \right) dx \\ &\geq \alpha_0 \int_\Omega (|\nabla u_\varepsilon^2 - |\nabla w|^2)\, dx\end{aligned}$$

implies

$$\|u_\varepsilon\|_{L^2(0,T;H^1)} \leq C < \infty.$$

This estimate and (3.6) imply ([L],[Si]) the compactness of the set $(u_\varepsilon,\ 1 \geq \varepsilon > 0)$ in the space $L^2(Q)$. Hence there is a sequence $\varepsilon_j \longrightarrow 0,\ (j \longrightarrow \infty)$ such that

$$u_{\varepsilon_j} \longrightarrow u \quad \text{in } L^2(Q), \quad u_{\varepsilon_j} \rightharpoonup u \quad \text{in } L^2(0,T;H^1).$$

Now, taking into account that the operator A is of variational type ([L]), we can take the limit $j \longrightarrow \infty$ and show that $v = f'(u) + w$ is solution of (3.3).

Uniqueness.
Let $v_i,\ i = 1,2,$ be solutions of (3.3) and $u_i = 1/(1+\exp(w - v_i))$. Define

$$d(t) = \int_\Omega \left\{ f(u_1) + f(u_2) - 2\, f\left(\frac{u_1+u_2}{2}\right) \right\} dx.$$

Then Lemma 3.2 yields (with $w_1 = w_2$)

$$\begin{aligned}d'(t) &= \left(u_{1t}, f'(u_1) - f'\left(\frac{u_1+u_2}{2}\right)\right) + \left(u_{2t}, f'(u_2) - f'\left(\frac{u_1+u_2}{2}\right)\right) \\ &= -\left(A(v_1,w), f'(u_1) - f'\left(\frac{u_1+u_2}{2}\right)\right) - \left(A(v_2,w), f'(u_2) - f'\left(\frac{u_1+u_2}{2}\right)\right) \\ &\leq \alpha_1 r_\infty^2 \|u_1 - u_2\|^2.\end{aligned}$$

By the strong convexity of f (see (2.4)) we have

$$\|u_1(t) - u_2(t)\|^2 \leq d(t) = \int_0^t d'(s)\, ds \leq \alpha_1 r_\infty^2 \int_0^t \|u_1(s) - u_2(s)\|^2 ds.$$

The uniqueness assertion $u_1(t) = u_2(t),\ t \geq 0,$ follows from Gronwall's lemma. □

To prove existence and uniqueness of solutions for the problem (2.7)–(2.9) we define an operator $\mathcal{B} \in (C([0,T];L^2) \mapsto C([0,T];L^2))$ by

$$\mathcal{B}u = \frac{1}{1+\exp(w - v(w))}, \tag{3.7}$$

where

$$w(t,x) = \int_\Omega \mathcal{K}(|x-y|)(1 - 2\,u(t,y))\, dy \tag{3.8}$$

and $v(w)$ is given by Lemma 3.3.

Lemma 3.4. *The operator* $\mathcal{B}$ *satisfies the contraction condition*

$$\|\mathcal{B}u_1 - \mathcal{B}u_2\|_\lambda \le \frac{1}{2}\left\|u_1 - u_2\right\|_\lambda \tag{3.9}$$

with respect to the norm

$$\|u\|_\lambda = \sup_{t\in[0,T]}\{e^{-\lambda t}\|u(t)\|\}, \quad \lambda = \frac{\alpha_1}{4}\max\left(r_\infty^2, \frac{\alpha_1\, r_2^2}{\alpha_0}\right).$$

Proof. Let $u_i \in L^\infty(Q)$, $i = 1,2$. We calculate the corresponding $w_i \in L^\infty(0,T;H^{1,\infty})$ from (3.8) and denote by v_i the solutions of (3.3), respectively. With the same arguments as in the uniqueness proof in Lemma 3.3 we get from Lemma 3.2

$$\|\mathcal{B}u_1(t) - \mathcal{B}u_2(t)\|^2 \le \int_0^t \frac{\alpha_1}{4}\left(r_\infty^2\|\mathcal{B}u_1(s) - \mathcal{B}u_2(s)\|^2 + \frac{\alpha_1}{8\alpha_0}\left\|\nabla(w_1 - w_2)\right\|^2\right) ds.$$

Because of

$$\|\nabla(w_1 - w_2)\|^2 \le \left\|2\int_\Omega \mathcal{K}(|x-y|)(u_1 - u_2)\, dy\right\|_{H^1}^2 \le 4r_2^2\|u_1 - u_2\|^2$$

we get

$$\begin{aligned}\|\mathcal{B}u_1(t) - \mathcal{B}u_2(t)\|^2 \;&\le\; \frac{\alpha_1}{4}\int_0^t \Big(r_\infty^2\|\mathcal{B}u_1(s) - \mathcal{B}u_2(s)\|^2 e^{-2\lambda s} \\ &\qquad + \frac{\alpha_1 r_2^2}{2\alpha_0}\left\|u_1(s) - u_2(s)\right\|^2 e^{-2\lambda s}\Big) e^{2\lambda s} ds \\ &\le\; \frac{\alpha_1}{4}\left(r_\infty^2\|\mathcal{B}u_1 - \mathcal{B}u_2\|_\lambda^2 + \frac{\alpha_1 r_2^2}{2\alpha_0}\left\|u_1 - u_2\right\|_\lambda^2\right)\int_0^t e^{2\lambda s} ds\end{aligned}$$

or

$$\|\mathcal{B}u_1(t) - \mathcal{B}u_2(t)\|^2 e^{-2\lambda t} \le \frac{\alpha_1}{8\lambda}\left(r_\infty^2\left\|\mathcal{B}u_1 - \mathcal{B}u_2\right\|_\lambda^2 + \frac{\alpha_1 r_2^2}{2\alpha_0}\left\|u_1 - u_2\right\|_\lambda^2\right).$$

Taking the supremum over $[0,T]$ on the left hand side and choosing $\lambda > 0$ so that

$$\frac{\alpha_1 r_\infty^2}{8\lambda} \le \frac{1}{2}, \quad \frac{\alpha_1 r_2^2}{16\alpha_0\lambda} \le \frac{1}{4}$$

we get (3.9). □

Theorem 3.5. *The problem* (2.7) – (2.9) *has a unique solution* (u,v,w) .

Proof. The operator $\mathcal{B}$ has a fixed point $u \in C([0,T],L^2)$ by Banach's fixed point theorem. Then, evidently, (u,v,w) with w given by (3.8) and v being the corresponding solution of (3.3) is solution of of (2.7)–(2.9). On the other hand, for any solution (u,v,w) the first component u must be fixed point of B and hence is unique. $\square$

Next we want to show a regularity result stating that under the additional assumption

$$0 < u_0(x) < 1, \quad x \in \Omega, \tag{3.10}$$

the function v belongs to $L^\infty(\Omega)$ globally in time.

Theorem 3.6. *Suppose* (3.10). *Then*

$$v \in L^\infty(Q) \cap L^2(0,T;H^1) \quad \textit{and} \quad 0 < u(t,x) < 1 \quad \textit{for a.a.} \quad (t,x) \in Q.$$

Proof. By assumption (ii) in Section 2

$$m_1 = \sup_{x\in\Omega} \int_\Omega \Big|\mathcal{K}(|x-y|)\Big|\, dy < \infty$$

and, consequently,

$$\|w\|_{L^\infty(Q)} \le m_1. \tag{3.11}$$

We introduce

$$u = \sigma(v-w) = \frac{1}{1+\exp(w-v)},$$

and have

$$\sigma'(v-w) = u(1-u) = \frac{\exp(w-v)}{(1+\exp(w-v))^2} = \frac{1}{f''(u)},$$

$$\sigma''(v-w) = \frac{(\exp(w-v)-1)\exp(w-v)}{(1+\exp(w-v))^3}.$$

Because of (3.11) we have

$$\sigma''(v-w) \le 0 \quad \text{if} \quad v \ge w, \tag{3.12}$$

$$\sigma''(v-w) \ge 0 \quad \text{if} \quad v \le w. \tag{3.13}$$

Using (3.12) and testing (2.8) with

$$h = \frac{\varphi^{r+1}}{\sigma'(v-w)}, \quad r>0, \quad \varphi = [v-w]_+ = \max(0, v-w),$$

we get ([GSk]) with $z = v-w$ after some calculation

$$\frac{1}{(r+2)}\frac{d}{dt}\int\limits_{v\ge w} \varphi^{r+2}dx + \int\limits_{v\ge w} a\nabla v\cdot\{(r+1)\,\varphi^r\nabla z - \sigma''(z)\,h\,\nabla z\}\,dx = 0. \tag{3.14}$$

We expand the integrand of the second integral on the left hand side in the form

$$\begin{aligned} S &= a(|v|)[\nabla z + \nabla w]\cdot\{(r+1)\,\varphi^r\nabla z - \sigma''(z)\,h\,\nabla z\} \\ &= a(|v|)(r+1)\,\varphi^r\{|\nabla z|^2 + \nabla w\cdot\nabla z\} - a(|v|)\sigma''(z)\,h\{|\nabla z|^2 + \nabla w\cdot\nabla z\}. \end{aligned}$$

Because of $\sigma''(z)\le 0$ for $v\ge w$ we can estimate

$$\begin{aligned} S \;\ge\;& a(|v|)(r+1)\,\varphi^r\Big\{|\nabla z|^2 - \frac{1}{2}\left(|\nabla w|^2 + |\nabla z|^2\right)\Big\} \\ & - a(|v|)\sigma''(z)\,h\Big\{|\nabla z|^2 - \frac{1}{2}\left(k|\nabla w|^2 + \frac{1}{k}|\nabla z|^2\right)\Big\}. \end{aligned}$$

From assumption (iii) in Section 2 we have $a(|v|)\ge\alpha_0$, and with the choice $k=1/2$ we get

$$S \ge \frac{\alpha_0}{2}(r+1)\,\varphi^r\,|\nabla z|^2 - \frac{1}{2}\,a(|v|)\,(r+1)\,\varphi^r\,|\nabla w|^2 + \frac{1}{4}\,a(|v|)\,\frac{\sigma''(z)}{\sigma'(z)}\,\varphi^{r+1}\,|\nabla w|^2.$$

Because of

$$-1 \le \frac{\sigma''(z)}{\sigma'(z)} \le 1$$

and $|a(|v|)|\le\alpha_1$ (Section 2, (iii)) and assumption (ii) we obtain

$$S \ge \frac{\alpha_0}{2}(r+1)\,\varphi^r\,|\nabla z|^2 - \frac{\alpha_1 r_\infty^2}{2}\,(r+1)\varphi^r - \frac{\alpha_1 r_\infty^2}{4}\,\varphi^{r+1}.$$

Taking into account that

$$\varphi^r|\nabla z_+|^2 = \frac{4}{(r+2)^2}\left|\nabla\left(z_+^{\frac{r+2}{2}}\right)\right|^2 = \frac{4\,|\nabla(\varphi^{\frac{r+2}{2}})|^2}{(r+2)^2},$$

we finally get from the identity (3.14) the estimate

$$\begin{aligned} \frac{1}{(r+2)}\frac{d}{dt}\int\limits_{v\ge w}\varphi^{r+2}dx \;\le\;& -\frac{2\alpha_0(r+1)}{(r+2)^2}\int_\Omega|\nabla(\varphi^{\frac{r+2}{2}})|^2dx \\ & + \frac{\alpha_1 r_\infty^2}{4}\int_\Omega\Big\{2(r+1)\varphi^r + \varphi^{r+1}\Big\}dx. \end{aligned}$$

By a technique due to N. Alikakos ([Al1], [Al2]) we conclude from this estimate that

$$\|\varphi\|_{L^\infty(Q)} \le C$$

for an appropriate constant C. With (3.11) this gives an upper bound for v:

$$v(x) \le m_1 + C \quad \text{for a.a } x\in\Omega. \tag{3.15}$$

Analogously, from (3.13) with the test function

$$h = \frac{\psi^{r+1}}{\sigma'(v-w)}, \quad r > 0, \quad \psi = -[v-w]_- = -\min(0, v-w)$$

and (3.11) we get a lower bound for v :

$$v(x) \geq -(m_1 + C) \quad \text{ for a.a } \ x \in \Omega. \tag{3.16}$$

From (3.15), (3.16) follows the assertion. □

4. Global behaviour

In this section we study the global behaviour of the solution of (2.1)–(2.3) for $T \longrightarrow \infty$. Our main tool is the fact (formulated in Lemma 3.1) that the free energy F is a Lyapunov functional. Therefore we have

$$\frac{d}{dt} F(u(t)) \ \leq \ -\alpha_0 \int_\Omega (u(1-u)|\nabla v|^2)(t)\, dx \ \leq \ 0, \tag{4.1}$$

$$\int_0^\infty \int_\Omega \frac{|\nabla v(t)|^2}{f''(u(t))}\, dx \ \leq \ C < \ \infty. \tag{4.2}$$

Theorem 4.1. *Let* (u, v, w) *be a solution of* (2.7) – (2.9). *Then there exist a sequence* $\{t_k, \ k = 1, 2, \ldots\}$ *with* $t_k \longrightarrow \infty$ *for* $k \longrightarrow \infty$ *and a tripel* (u^*, v^*, w^*) *such that* $u_k = u(t_k),\ v_k = v(t_k),\ w_k = w(t_k)$ *satisfy*

$$u_k \longrightarrow u^* \quad \textit{strongly in } L^2 \ \textit{ and weakly in } \ H^1, \tag{4.3}$$

$$w_k \longrightarrow w^* \quad \textit{strongly in } \ H^1, \tag{4.4}$$

$$\arctan\left(e^{-v_k/2}\right) \longrightarrow \arctan\left(e^{-v^*/2}\right) \quad \textit{strongly in } \ H^1, \ \ v^* = const. \tag{4.5}$$

Moreover, the following relations hold:

$$w^*(x) = \int_\Omega \mathcal{K}(|x-y|)(1 - 2\, u^*(y))\, dy, \quad \int_\Omega u^* dx = u_\alpha |\Omega|, \tag{4.6}$$

$$u^* = \frac{1}{1 + \exp(w^* - v^*)}, \quad v^* = const. \tag{4.7}$$

Proof. By (4.2) there exists a sequence $t_j \in [j, j+1],\ j = 1, 2, \ldots$, such that $u_j = u(t_j),\ v_j = v(t_j),\ w_j = w(t_j)$ satisfy

$$\lim_{j \to \infty} \int_\Omega \frac{|\nabla v_j|^2}{f''(u_j)}\, dx = 0. \tag{4.8}$$

With

$$\nabla u = \frac{\nabla(v-w)}{f''(u)} \quad \text{and} \quad \frac{1}{f''(u)} = u(1-u) \leq \frac{1}{4} \quad \text{for} \quad 0 \leq u \leq 1$$

and with assumption (ii) in Section 2 and (4.8) we get

$$\int_\Omega |\nabla u_j|^2 dx = \int_\Omega \left(\frac{|\nabla(v_j - w_j)|}{f''(u_j)} \right)^2 dx \le 2 \int_\Omega \frac{|\nabla v_j|^2 + |\nabla w_j|^2}{(f''(u_j))^2} dx$$

$$\le \frac{1}{2} \int_\Omega \frac{|\nabla v_j|^2}{f''(u_j)} dx + \frac{1}{8} \int_\Omega |\nabla w_j|^2 dx \ \le \ \varepsilon + \frac{r_2^2 |\Omega|^2}{8} \ = \ C.$$

Hence by the compactness of the embedding $H^1 \subset L^2$ there exists a subsequence $\{t_k\} \subset \{t_j\}$ such that (4.3) holds. Again by assumption (ii) in Section 2 the convergence (4.4) and

$$\|w_k\|_{L^\infty} \le C$$

follows. This implies

$$\int_\Omega \left| \nabla \arctan \left(e^{-v_k/2} \right) \right|^2 dx = \frac{1}{4} \int_\Omega \frac{|\nabla v_k|^2 \, e^{-v_k}}{(1 + e^{-v_k})^2} dx \le C \int_\Omega \frac{|\nabla v_k|^2}{f''(u_k)} dx \longrightarrow 0$$

and consequently (4.5). Finally, (4.3)–(4.5) together with (2.7), (2.9), (2.10) and assumption (iv) (Section 2) give (4.6), (4.7). □

In view of the regularity result in Theorem 3.6, we formulate:

Remark 4.1. From the finiteness of v^* follows $0 < u^* < 1$, even if the set

$$\{x \in \Omega |\ u_0(x) = 0 \quad \text{or} \quad u_0(x) = 1\}$$

has positive measure.

Remark 4.2. Lemma 3.1 and Theorem 4.1 imply, together with Lebesgue's dominated convergence theorem,

$$\lim_{t \to \infty} F(u(t)) = F(u^*), \quad u^* = \frac{1}{1 + \exp(w^* - v^*)} \ .$$

However, it is an open problem whether

$$u(t) \longrightarrow u^*, \quad w(t) \longrightarrow w^* \qquad \text{as } t \longrightarrow \infty$$

(and not only along a subsequenc $\{t_k\}$).

The system (4.6) can be considered as Euler – Lagrange equation of an appropriate restricted minimum problem.

Proposition 4.2. *Let* (u^*, v^*, w^*) *be a solution of* (4.6), (4.7). *Then* $z^* = w^* - v^*$ *is minimizer of the minimum problem*

$$\mathcal{G}(z) = F\left(\frac{1}{1 + e^z} \right) \longrightarrow \min \tag{4.9}$$

with the constraint

$$\int_\Omega \frac{dx}{1+e^z} = u_\alpha |\Omega|,$$

where F *is the free energy*

$$F\left(\frac{1}{1+e^z}\right) = \int_\Omega \Big\{ z\left(1-\frac{1}{1+e^z}\right) - \log(1+e^z)$$
$$+\frac{1}{1+e^z}\int_\Omega \mathcal{K}(|x-y|)\left(1-\frac{1}{1+e^{z(y)}}\right)dy\Big\}dx.$$

Proof. We have to show that the variational (Gâteaux –) derivative vanishes:

$$\frac{d}{ds}\mathcal{G}(z^*+sh)\Big|_{s=0} = 0 \tag{4.10}$$

for all $h \in L^\infty$ satisfying

$$\frac{d}{ds}\int_\Omega \frac{dx}{1+e^{z^*+sh}}\Big|_{s=0} = \int_\Omega \frac{he^{z^*}}{(1+e^{z^*})^2}\,dx = 0, \tag{4.11}$$

which takes into account the constraint. We find

$$\frac{d}{ds}\mathcal{G}(z+sh)\Big|_{s=0} = \int_\Omega \Big\{ \frac{(he^z+zhe^z)(1+e^z)-zhe^{2z}}{(1+e^z)^2} - \frac{he^z}{1+e^z}$$
$$-\frac{h(x)e^{z(x)}}{(1+e^{z(x)})^2}\int_\Omega \mathcal{K}(|x-y|)\frac{e^{z(y)}}{(1+e^{z(y)})}\,dy$$
$$+\frac{1}{1+e^{z(x)}}\int_\Omega \mathcal{K}(|x-y|)\frac{h(y)e^{z(y)}}{(1+e^{z(y)})^2}dy\Big\}dx$$
$$= \int_\Omega \Big\{ \frac{he^z}{(1+e^z)^2}\Big(z+\int_\Omega \mathcal{K}(|x-y|)\frac{1-e^{z(y)}}{1+e^{z(y)}}dy\Big)\Big\}dx.$$

Setting $z = z^* = w^* - v^*$, using (4.6), (4.7) and (4.11) we get (4.10). □

From Theorem 4.1 and Proposition 4.2 we conclude:

Theorem 4.3. *Let* (u,v,w) *be the solution to* (2.7)–(2.7). *Then there is a sequence* $\{t_k,\ k=1,2,\ldots\}$ *with* $t_k \longrightarrow \infty$ *for* $k \longrightarrow \infty$ *such that* $z_k = w(t_k) - v(t_k)$ *converges in* H^1 *strongly to a minimizer of* (4.9).

5. Newton kernel and chemotaxis

In this section we specify $\mathcal{K}$ in (2.1) as the Newton kernel

$$\mathcal{K}(|x|) = \frac{\kappa}{|x|},\quad \kappa = \frac{1}{4\pi},\quad n=3.$$

It turns out that in this case the alternative Cahn – Hilliard system (2.1), (2.2) is similar to the chemotaxis model of Keller – Segel ([KS]). Indeed, as a well–known fact of potential theory the potential

$$w(x) = \kappa \int_\Omega \frac{(1 - 2\,u(y))}{|x-y|}\,dy$$

satisfies Poisson's equation

$$-\Delta w = 1 - 2\,u.$$

After adjusting boundary values by the ansatz

$$w = w_0 + \omega$$

with

$$-\Delta w_0 = 1 - 2\,u_\alpha \quad \text{in } \Omega, \quad \nu \cdot \nabla w_0 = \nu \cdot \nabla w \quad \text{on } \Gamma,$$

we can determine ω as solution of the problem

$$-\Delta\,\omega = 2\,(u_\alpha - u) \quad \text{in } \Omega, \quad \nu \cdot \nabla \omega = 0 \quad \text{on } \Gamma, \quad \int_\Omega \omega\,dx = 0. \tag{5.1}$$

Now we can rewrite (2.2) as

$$\begin{cases} \dfrac{\partial u}{\partial t} - \nabla \cdot \Big\{ a\,(\nabla u + u\,(1-u)\,\nabla(w_0 + \omega)) \Big\} = 0 \quad \text{in } Q, \\ \nu \cdot (\nabla u + u\,(1-u)\,\nabla w_0) = 0 \quad \text{on } \Gamma_T. \end{cases} \tag{5.2}$$

The system (5.1), (5.2) coincides substantially with models of chemotaxis ([GZ]).

In view of Section 4 equilibrium states of (5.1), (5.2) are solutions of the nonlinear nonlocal boundary value problem

$$-\Delta\,\omega = 2\left(u_\alpha - \frac{1}{1+\gamma\exp(\omega + w_0)}\right) \quad \text{in } \Omega, \quad \nu \cdot \nabla\omega = 0 \quad \text{on } \Gamma, \tag{5.3}$$

$$\int_\Omega \omega\,dx = 0, \quad \int_\Omega \frac{dx}{1+\gamma\exp(\omega + w_0)} = u_\alpha|\Omega|. \tag{5.4}$$

The system (5.3), (5.4) can be understood as the Euler – Lagrange equation of the minimum problem

$$\mathcal{E}(\omega) = \int_\Omega \left(\frac{|\nabla\omega|^2}{2} - 2u_\alpha\omega + 2\log\left(\frac{\exp(\omega + w_0)}{1+\gamma\exp(\omega + w_0)}\right)\right) dx \longrightarrow \min$$

under the constraints (5.4).

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