Double Obstacle Limit for a Navier-Stokes/Cahn-Hilliard System

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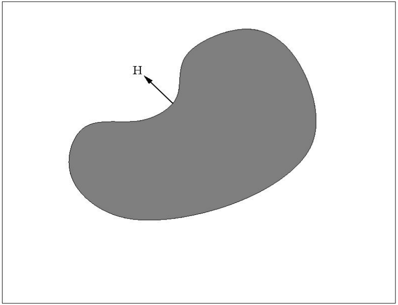
Diffuse Interface Models

We consider two (macroscopically) immiscible incompressible, viscous fluids like oil and water.

Classical Models: Interface is a two-dimensional surface.

Surface tension is proportional to the mean curvature.



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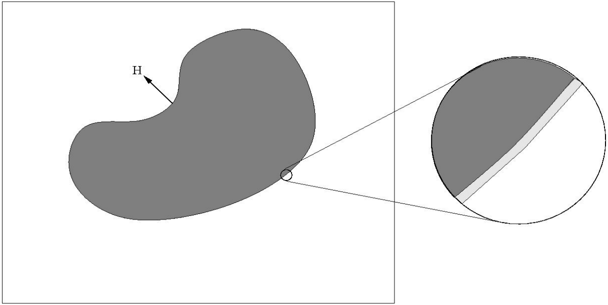


But: Sharp Interface is an idealization (van der Waals).

Fluid mix in a thin interfacial region.

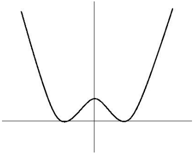
Phase Separation/Cahn-Hilliard Equation

We consider two partly miscible components, e.g. Al-/Ni-atoms in a melted alloy, oil and water.
Let $c_j \colon \Omega \to \mathbb{R}$ be the concentration of the component $j = 1, 2$, $c = c_1 - c_2$, and let

$$E_\varepsilon(c) = \frac{\varepsilon}{2} \int_\Omega |\nabla c(x)|^2 \, dx + \varepsilon^{-1} \int_\Omega f(c(x)) \, dx$$

be the free energy of the mixture, where $\Omega \subseteq \mathbb{R}^d$, $d = 1, 2, 3$, $\varepsilon > 0$ and

$$f \colon \mathbb{R} \to [0, \infty) \text{ with } f(c) = 0 \Leftrightarrow c = \pm 1.$$



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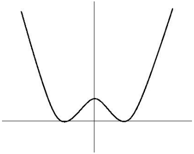

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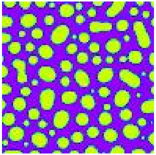
H^{-1}-gradient flow of E_ε describes dynamics of phase separation:



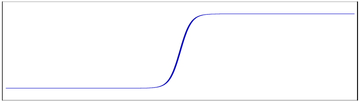
$$\partial_t c = \Delta \mu \qquad \text{in } \Omega \times (0, \infty) \qquad (1)$$

$$\mu = \varepsilon^{-1} f'(c) + \varepsilon \Delta c \qquad \text{in } \Omega \times (0, \infty) \qquad (2)$$

Choice of Free Energy Density(I)

Typical choice: Smooth double well potential as e.g. $f(c) = \frac{1}{8}(1 - c^2)^2$.
Then the optimal profile of a diffuse interface is

$$c_0(x) = \tanh \frac{x}{2\varepsilon}, \qquad x \in \mathbb{R},$$



which minimizes E_ε in the case $\Omega = \mathbb{R}$ with constraint $c(x) \to_{x \to \pm\infty} \pm 1$.
Note: $c_0(x) \in (-1, 1)$ for all $x \in \mathbb{R}$.

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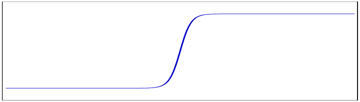

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Note: $c_0(x) \in (-1,1)$ for all $x \in \mathbb{R}$.

Problem: For smooth f solutions $c(x,t)$ of Cahn-Hilliard system

$$\begin{aligned} \partial_t c &= \Delta\mu && \text{in } \Omega\times(0,\infty) \\ \mu &= \varepsilon^{-1} f'(c) + \varepsilon\Delta c && \text{in } \Omega\times(0,\infty) \end{aligned}$$

might not stay in $[-1,1]$!

Choice of Free Energy (II)

In the following we consider the logarithmic free energy density

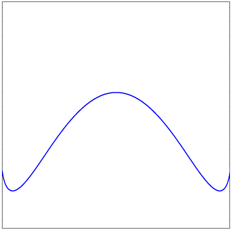
$$f_\theta(c) = \begin{cases} \theta((1-c)\log(1-c) + (1+c)\log(1+c)) - \theta_c c^2, & \text{if } c \in [-1,1], \\ +\infty & \text{else.} \end{cases}$$

for some $0 < \theta < \theta_c$ and $\nu(c) > 0$ on $[-1,1]$, cf. Cahn & Hilliard '58, Elliott & Luckhaus '91.

Note:

$$f_\theta(c) = \underbrace{\theta\varphi(c)}_{\text{convex}} - \frac{\theta_c}{2}c^2$$

$$f'_\theta(c) \to_{c\to\pm1} \pm\infty$$

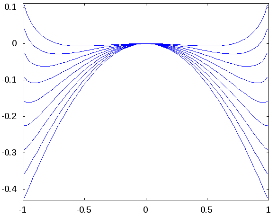


Elliott & Luckhaus '91, Debussche & Dettori '95, Kenmochi et al. '95: Existence of unique solutions of (1)-(2) such that $c(x,t) \in (-1,1)$. Alternative proofs: Miranville & Zelik '04, A. & Wilke '07

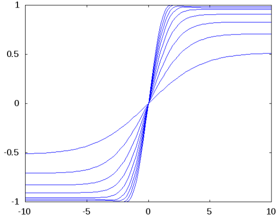
Double Obstacle/Deep Quench Limit (I)

We have

$$f_\theta(c) \to_{\theta\to 0} f_0(c) = \mathbf{I}_{[-1,1]}(c) - \frac{\theta_c}{2}c^2, \quad \mathbf{I}_{[-1,1]}(c) := \begin{cases} 0 & \text{if } c \in [-1,1], \\ +\infty & \text{else.} \end{cases}$$



Graph of $f_\theta(c)$, $\theta = 0.9, 0.8, \ldots, 0.1$



Optimal profile $\theta = 0.9, 0.8, \ldots, 0.1$

The optimal profile for E_ε with f_0 and $\varepsilon = \theta_c = 1$ is

$$c_0(x) = \begin{cases} -1 & \text{if } c < -\frac{\pi}{2} \\ \sin x & \text{if } c \in [-\frac{\pi}{2}, \frac{\pi}{2}] \\ 1 & \text{if } c > \frac{\pi}{2} \end{cases}$$

Double Obstacle/Deep Quench Limit (II)

The optimal profile

$$c_0(x) = \begin{cases} -1 & \text{if } c < -\frac{\pi}{2} \\ \sin x & \text{if } c \in [-\frac{\pi}{2}, \frac{\pi}{2}] \\ 1 & \text{if } c > \frac{\pi}{2} \end{cases}$$

solves the differential inclusion

$$c''(x) + c(x) \in \partial I_{[-1,1]}(c(x)) = \begin{cases} (-\infty, 0] & \text{if } c(x) = -1 \\ \{0\} & \text{if } c(x) \in (-1,1) \\ [0,\infty) & \text{if } c(x) = 1 \\ \emptyset & \text{else} \end{cases}$$

Elliott & Luckhaus '91: Solutions of Cahn-Hilliard system (1)-(2) with f_θ converge as $\theta \to 0$ to solution of

$$\begin{aligned} \partial_t c &= \Delta\mu && \text{in } \Omega \times (0,T) \\ \mu + \varepsilon\Delta c + \varepsilon^{-1}\theta_c c &\in \partial I_{[-1,1]}(c(x)) && \text{in } \Omega \times (0,T) \end{aligned}$$

Diffuse Interface Model in the Case of Matched Densities

If the densities of the fluids are the same, then one can derive:

$$\partial_t v + v\cdot\nabla v - \underbrace{\operatorname{div}(\nu(c)Dv)}_{\text{inner friction}} + \nabla p = \underbrace{-\varepsilon \operatorname{div}(\nabla c\otimes\nabla c)}_{\text{surface tension}} \quad \text{in } \Omega\times(0,\infty) \quad (3)$$

$$\operatorname{div} v = 0 \quad \text{in } \Omega\times(0,\infty) \quad (4)$$

$$\partial_t c + v\cdot\nabla c = m\Delta\mu \quad \text{in } \Omega\times(0,\infty) \quad (5)$$

$$\mu = -\varepsilon\Delta c + \varepsilon^{-1} f_\theta'(c) \quad \text{in } \Omega\times(0,\infty) \quad (6)$$

where $Dv = \frac{1}{2}(\nabla v + \nabla v^T)$, $\Omega\subset\mathbb{R}^d$ is a bounded smooth domain, together with boundary and initial conditions.

Derivation: Hohenberg & Halperin '74, Gurtin et al. '96

Analytical results: Starovoitov '93, Boyer '03, X. Feng '06, A. '07/'09

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Energy dissipation: For sufficiently smooth solutions we have

$$\frac{d}{dt} E(c(t), v(t)) = -\int_\Omega \nu(c)|Dv|^2\,dx - \int_\Omega m|\nabla\mu|^2\,dx \quad \text{with}$$

$$E(c(t), v(t)) = \frac{\varepsilon}{2}\int_\Omega |\nabla c(x)|^2\,dx + \varepsilon^{-1}\int_\Omega f_\theta(c(x))\,dx + \int_\Omega \frac{|v(t)|^2}{2}\,dx$$

Theorem (Existence, Regularity, Uniqueness, A. '07/'09)

Let $d = 2, 3$, $\theta > 0$. *For every* $v_0 \in L^2_\sigma(\Omega)$, $c_0 \in H^1(\Omega)$ *with* $E(c_0, v_0) < \infty$ *there is a weak solution* (v, c, μ) *of (3)-(6), which satisfies*

$$(v, \nabla c) \in L^\infty(0, \infty; L^2(\Omega)), \quad (\nabla v, \nabla \mu) \in L^2(0, \infty; L^2(\Omega)),$$
$$\nabla^2 c, f'_\theta(c) \in L^2_{loc}([0, \infty); L^6(\Omega)).$$

In particular, $c(t, x) \in (-1, 1)$ *a.e. Moreover,* $c \in BUC([0, \infty); W^1_q(\Omega))$ *with* $q > d$. *For* (v_0, c_0) *sufficiently smooth:*

1. *If* $d = 2$*, then the weak solution is unique and regular.*
2. *If* $d = 3$*, there are some* $0 < T_0 < T_1 < \infty$ *such that the weak solution is regular and (locally) unique on* $(0, T_0)$ *and* $[T_1, \infty)$*.*

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Theorem (Uniform Bounds, A. '09)

The solutions $(v, c, \mu) = (v^\theta, c^\theta, \mu^\theta)$, $\theta \in (0, 1)$ *are uniformly bounded in the function spaces above.*

Structure of the Proof

First study the separate systems:

1. Cahn-Hilliard equation with convection and singular potential (based on $E_\varepsilon(c) = E_{0,\theta}(c) - \frac{\theta_c}{2}\|c\|_2^2$ with $E_{0,\theta}$ convex)
2. (Navier-)Stokes system with variable viscosity

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Existence of weak solutions:

Approximation and compactness argument

Higher Regularity: Use regularity results for separate systems

Uniqueness: Gronwall's inequality once $c \in L^\infty(0, T; C^1(\overline{\Omega}))$ and $v \in L^\infty(0, T; W^1_s(\Omega))$, $s > d$.

Crucial ingredient for higher regularity:

A priori estimate for $c \in BUC([0, \infty); W^1_q(\Omega))$, $q > d$!

A priori Estimates for c

W^2_r-estimate for c: Formally multiply

$$\mu(x,t) = -\Delta c(x,t) + f_\theta'(c(x,t))$$

by $f_\theta'(c(x,t)) = \theta\varphi'(c(x,t)) - \theta_c c(x,t)$ to obtain

$$\int_\Omega f_\theta'(c(t))^2\,dx + \int_\Omega \underbrace{f_\theta''(c(t))}_{\geq -\theta_c} |\nabla c(t)|^2\,dx \leq C\|\mu(t)\|_2$$

uniformly in $\theta > 0$.

A priori Estimates for c

W^2_r-estimate for c: Formally multiply

$$\mu(x,t) = -\Delta c(x,t) + f'_\theta(c(x,t))$$

by $f'_\theta(c(x,t)) = \theta\varphi'(c(x,t)) - \theta_c c(x,t)$ to obtain

$$\int_\Omega f'_\theta(c(t))^2\,dx + \int_\Omega \underbrace{f''_\theta(c(t))}_{\geq -\theta_c} |\nabla c(t)|^2\,dx \leq C\|\mu(t)\|_2$$

uniformly in $\theta > 0$. Similarly, for $2 \leq r < \infty$

$$\|f'_\theta(c(t))\|_r + \|c(t)\|_{W^2_r} \leq C_r\left(\|\mu(t)\|_r + \|\nabla c(t)\|_2\right).$$

$$\Rightarrow c \in L^2_{\mathrm{uloc}}([0,\infty); W^2_6(\Omega))$$

where

$$\|c\|_{L^2_{\mathrm{uloc}}([0,\infty);X)} = \sup_{t\geq 0}\|c\|_{L^2(t,t+1;X)}.$$

Modifications: Higher regularity in time in Besov spaces.

Higher Time Regularity for c

$L^\infty(0,\infty;H^{-1}_{(0)})$-estimate of $\partial_t c$: Multiplying

$$\partial_t^2 c + \Delta(\Delta c - \underbrace{f''(c)}_{\geq -\theta_c}\partial_t c) = -\partial_t(v\cdot\nabla c)$$

by $-\Delta_N^{-1}\partial_t c$ yields

$$\|\partial_t c\|_{L^\infty(0,\infty;H^{-1}_{(0)})} + \|\nabla\partial_t c\|_{L^2(Q)} \leq C(c_0)\left(1+\|\partial_t v\|_{L^{\frac{4}{3}}_{\mathrm{uloc}}(0,\infty;V_n')}\right)$$

where $V_n(\Omega) = \{\varphi\in H^1(\Omega)^n : n\cdot\varphi|_{\partial\Omega} = 0\}$.

$\Rightarrow \mu\in L^\infty(0,\infty;H^1(\Omega))$

$\Rightarrow c\in L^\infty(0,\infty;W^2_r(\Omega))$, $r=6$ if $d=3$ and $1<r<\infty$ if $d=2$.

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Problem: In general $\partial_t v \in L^{\frac{4}{3}}_{\mathrm{uloc}}(0,\infty; H^{-1}(\Omega)^n) \not\subseteq L^{\frac{4}{3}}_{\mathrm{uloc}}(0,\infty; V_n')$!
Solution: Replace $\partial_t c$ by $h^{-\tau}\Delta_h c$. Use $v \in B^\tau_{\frac{4}{3}\infty;\mathrm{uloc}}([0,\infty); H^{-s}(\Omega))$
with $0 < s < \frac{1}{2}$, $\tau > \frac{2}{3}$ as well as $H^s_0(\Omega) = H^s(\Omega)$ and $H^{-s}(\Omega) = H^s(\Omega)'$.
... $\Rightarrow c \in BUC([0,\infty); W^1_q(\Omega))$, $q > 3$.

Theorem (Double Obstacle Limit, A.'09)

There a subsequence of $(v^\theta, c^\theta, \mu^\theta)_{\theta\in(0,1)}$ *converges to* (v^0, c^0, μ^0) *solving*

$$\partial_t v + v\cdot\nabla v - \operatorname{div}(\nu(c)Dv) + \nabla p = \mu_0 \nabla c \quad \text{in } \Omega\times(0,\infty) \tag{7}$$

$$\operatorname{div} v = 0 \quad \text{in } \Omega\times(0,\infty) \tag{8}$$

$$\partial_t c + v\cdot\nabla c = m\Delta\mu \quad \text{in } \Omega\times(0,\infty) \tag{9}$$

$$b := \mu + \varepsilon\Delta c + \varepsilon^{-1}\theta_c c \in \partial I_{[-1,1]}(c) \quad \text{in } \Omega\times(0,\infty) \tag{10}$$

and $c(x,t)\in[-1,1]$ *for all* $(x,t)\in\Omega\times(0,\infty)$. *Moreover,*

$$(v^0,\nabla c^0)\in L^\infty(0,\infty;L^2(\Omega)), \quad (\nabla v^0,\nabla\mu^0)\in L^2(0,\infty;L^2(\Omega)),$$
$$\nabla^2 c^0, b\in L^2_{loc}([0,\infty);L^6(\Omega)),\ c^0\in BUC([0,\infty);W^1_q(\Omega)), q>d$$

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Open Questions

Question: How much does $\theta \geq 0$ influences the Ostwald ripening effect (for fixed ε)?

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Simulation by S. Bartels

Question: Does $(v(t), c(t))$ converges to stationary solution as $t \to \infty$ if $\theta = 0$? (Known for $\theta > 0$, A. '07/'09)