Phase Separation in Heterogeneous Media

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Overview

- Brief Introduction to Cahn-Hilliard
- Phase Transitions of Heterogeneous Media, The Critical Case $\varepsilon \sim \delta$ and Fixed Wells – Riccardo Cristoferi, IF, Adrian Hagerty, and Cristina Popovici (2019, 2020)
- Phase Transitions of Heterogeneous Media, The Supercritical Case $\delta \ll \varepsilon$ and Fixed Wells – Riccardo Cristoferi, IF, Likhit Ganedi (2023, submitted)
- Phase Transitions of Heterogeneous Media, The Subcritical Case $\varepsilon \ll \delta$, Moving Wells and Fixed Wells– Riccardo Cristoferi, IF, Likhit Ganedi (2022 to appear, and in progress)
- What is next, and open problems ...

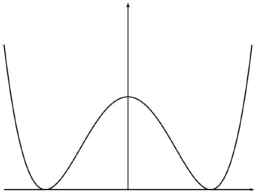
Brief Introduction to Cahn-Hilliard

Van Der Waals (1893), Cahn and Hilliard (1958), Gurtin (1987)

Equilibrium behavior of a fluid with two stable phases ... described by the Gibbs free energy

$$I(u) := \int_\Omega W(u)\,dx$$

$W : \mathbb{R} \to [0, +\infty)$ ... double well potential



$W(u) := (1 - u^2)^2$, $\{W = 0\} = \{-1, 1\}$

- $\Omega \subset \mathbb{R}^N$ open ($N \geqslant 2$), bounded, container
- $u : \Omega \to \mathbb{R}$ density of a fluid
- $\int_\Omega u\,dx = m \ldots m$ total mass of the fluid
- W double-well potential energy per unit volume
- $W^{-1}(\{0\}) = \{a, b\} \ldots a < b$ two phases of the fluid

Problem

Minimize total energy

$$I(u) = \int_\Omega W(u)\,dx$$

subject to $\int_\Omega u\,dx = m$

Solution

Assume $|\Omega| = 1$ *and* $a < m < b$. *Then minimizers are of the form*

$$u_E(x) = \begin{cases} a & \text{if } x \in E, \\ b & \text{if } x \in \Omega \setminus E, \end{cases}$$

where $E \subseteq \Omega$ *is any measurable set with* $|E| = \frac{b-m}{b-a}$

NONUNIQUENESS OF SOLUTIONS

Selection via singular perturbations:

$$I_\varepsilon(u) := \int_\Omega \left[W(u) + \frac{\varepsilon^2}{2} |\nabla u|^2 \right] dx, \quad u \in C^1(\Omega), \varepsilon > 0$$

$\frac{\varepsilon^2}{2} \int_\Omega |\nabla u|^2 \, dx$ ... surface energy penalization

Gurtin's Conjecture

$$I_\varepsilon(u) := \int_\Omega \left[W(u) + \frac{\varepsilon^2}{2} |\nabla u|^2 \right] dx, \quad u \in C^1(\Omega)$$

$\{W = 0\} = \{a, b\}$

"Preferred" minimizers u_ε of

$$\min \left\{ I_\varepsilon(u) : \, u \in C^1(\Omega), \quad \int_\Omega u \, dx = m \right\}$$

converge to u_{E_0}, where

$$\mathrm{Per}_\Omega(E_0) \leqslant \mathrm{Per}_\Omega(E)$$

over all sets of finite perimeter $E \subseteq \Omega$ with $|E| = \frac{b-m}{b-a}$

Modica-Mortola, 1977

Asymptotic behavior of minimizers to I_ε described via Γ-convergence. Scaling by ε^{-1} yields

$$\mathcal{F}_\varepsilon := \varepsilon^{-1} I_\varepsilon \xrightarrow{\Gamma} \mathcal{F},$$

$$\mathcal{F}(u) := \begin{cases} c_W \ \ \mathrm{Per}_\Omega(A_0) & u \in BV(\Omega; \{a,b\}), \\ +\infty & u \in L^1(\Omega) \setminus BV(\Omega; \{a,b\}) \end{cases}$$

where

$$A_0 := \{u(x) = a\},\ c_W := \sqrt{2} \int_a^b \sqrt{W(s)}ds$$

$$\mathcal{F}_\varepsilon(u) := \frac{1}{\varepsilon} I_\varepsilon(u) = \int_\Omega \left[\frac{1}{\varepsilon} W(u) + \frac{\varepsilon}{2} |\nabla u|^2 \right] dx$$

$\mathcal{F}_\varepsilon$ and I_ε have the same minimizers

Γ-Convergence of Energy Functionals

Recall that a sequence of energy functionals $\mathcal{F}_\varepsilon : X^\varepsilon \to \mathbb{R}$ Γ-converges (with respect to the topology τ) to a limiting functional $\mathcal{F} : Y \to \mathbb{R}$ if

- For any $u_\varepsilon \xrightarrow{\tau} u \in Y$, we have

$$\mathcal{F}(u) \leqslant \liminf_{\varepsilon \to 0} \mathcal{F}_\varepsilon(u_\varepsilon).$$

- For any $u \in Y$, there exists $u_\varepsilon \in X^\varepsilon$ with $u_\varepsilon \xrightarrow{\tau} u$ and

$$\mathcal{F}(u) \geqslant (=) \limsup_{\varepsilon \to 0} \mathcal{F}_\varepsilon(u_\varepsilon).$$

Upshot: global minimizers of $\mathcal{F}_\varepsilon$ converge to global minimizers of $\mathcal{F}$.

So ... if we know the Γ-limit of $\{F_\varepsilon\}$ then we have a selection criterium: preferred minimizers of the original problem are minimizers of the Γ-limit $\mathcal{F}$

$$\mathcal{F}_\varepsilon(u) = \int_\Omega \left[\frac{1}{\varepsilon} W(u) + \frac{\varepsilon}{2}|\nabla u|^2\right] dx, \quad u \in W^{1,2}(\Omega)$$

Theorem

$\mathcal{F}_\varepsilon \xrightarrow{\Gamma} \mathcal{F}$ *with respect to strong convergence in* $L^1(\Omega)$, *where*

$$\mathcal{F}(u) := \begin{cases} c_W \operatorname{Per}_\Omega\left(u^{-1}(\{a\})\right) & \text{if } u \in BV(\Omega;\{a,b\}), \int_\Omega u\, dx = m, \\ +\infty & \text{otherwise} \end{cases}$$

$$c_W := \sqrt{2}\int_a^b \sqrt{W(s)}\, ds$$

<u>A non-exhaustive list of references</u>:

- Modica (1987)
- Sternberg (1988)
- Kohn and Sternberg (1989) – local minimizers via Γ-convergence
- IF and Tartar (1989) – vectorial setting, at least linear growth at infinity
- Bouchitté (1990) – coupled perturbations of the form (scalar-valued case) $\frac{1}{\varepsilon}\int_\Omega W(x, u, \varepsilon\nabla u)dx$, moving wells
- Baldo (1990)– multiple phases
- Ambrosio (1990)– phases are compact sets
- Owen and Sternberg (1991), Barroso and IF (1994)
- IF and Popovici (2005)– coupled perturbations of the form (vector-valued case) $\frac{1}{\varepsilon}\int_\Omega W(x, u, \varepsilon\nabla u)dx$
- Conti, IF, Leoni (2002)– higher order Modica-Mortola type $\int_\Omega \left[\frac{1}{\varepsilon}W(\nabla u) + \varepsilon|\nabla^2 u|^2\right] dx$
- ...

…Modern technologies, such as temperature-responsive polymers, take advantage of engineered inclusions.

Heterogeneities of the medium are exploited to obtain novel composite materials with specific physical properties.

To model such situations by using a variational approach based on the gradient theory, the potential and the wells have to depend on the spatial point, even in a discontinuous way.

Phase Transitions of Heterogeneous Media

Mixture depending on position . . . Lipid Rafts . . . within the cell membrane there are many coexisting fluid phases
Experimental: phase separation occurs at the scale of nanometers, there is no macroscopic phase separation, thermal fluctuations play a role in the formation of nanodomains

- Simons and Ikonen (1997) proposed that proteins move along the cell membrane through "Lipid Rafts" by a chemical reaction between the lipids and cholesterol

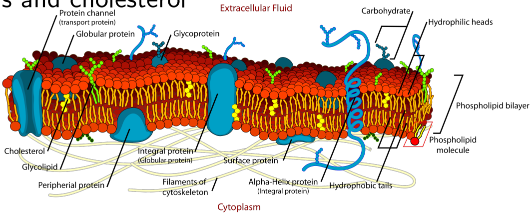


Figure: Cell Membrane– (Source: Wikipedia)

Lipid Rafts

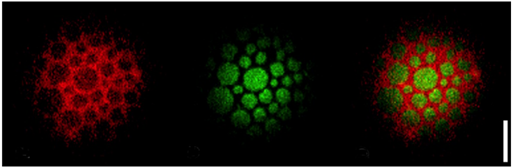


Figure: Fluorescent Imaging of Micron-scale fluid-fluid phase separation in giant unilamellar vesicles– Sengu

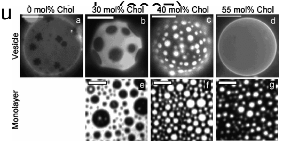


Figure: Macroscopic phase separation in a model membrane seeming to transition to a homogeneous material – Veatch and Keller (2002)

Modeling Considerations

- Assume all physiological parameters dependent on position
- Several different types of lipid rafts (so potentially different phases preferred at different positions)
- Use techniques of periodic homogenization to homogenize the submicroscopic phase separation into a macroscopic model

Fluids that exhibit periodic heterogeneity at small scales

$$\mathcal{F}_\varepsilon(u) := \int_\Omega \left[\frac{1}{\varepsilon} W\left(\frac{x}{\delta(\varepsilon)}, u \right) + \frac{\varepsilon}{2} |\nabla u|^2 \right] dx$$

where ... preferred phases are encoded in

$$W : \mathbb{R}^N \times \mathbb{R}^d \to [0, +\infty), N \geqslant 2, d \geqslant 1, \quad W(x,p) = 0 \iff p \in \{a(x), b(x)\},$$

$$W(\cdot, p) \text{ is } Q\text{-periodic for every } p,$$

and

$$\delta(\varepsilon) \to 0 \text{ as } \varepsilon \to 0.$$

Example: $W(x,p) = \chi_E(x) W_1(p) + \chi_{Q \setminus E} W_2(p)$
... shouldn't ask more than measurability w.r.t. x ...

Goal: Identify Γ-limit of $\mathcal{F}_\varepsilon$

Sharp Interface Limit for Heterogeneous Phases (wells at $a(x)$ and $b(x)$) Without Homogenization

- Bouchitté (1990) . . . a sharp interface limit in the scalar case
- Cristoferi and Gravina (2021) . . . vectorial case under strict assumptions on the behavior near the wells

So start with fixed wells:

$$W : \mathbb{R}^N \times \mathbb{R}^d \to [0, +\infty), N \geqslant 2, d \geqslant 1, \quad W(x, p) = 0 \iff p \in \{a, b\},$$

The Critical Case $\delta(\varepsilon) = \varepsilon$ and Fixed Wells : Riccardo Cristoferi, IF, Adrian Hagerty, and Cristina Popovici (2019, 2020)

Theorem (R. Cristoferi, IF , A. Hagerty, C. Popovici, *Interfaces Free Bound.*(2019, 2020))

Let $\delta(\varepsilon) = \varepsilon$. *Then* $\mathcal{F}_\varepsilon \xrightarrow{\Gamma} \mathcal{F}$,

$$\mathcal{F}(u) := \begin{cases} \displaystyle\int_{\partial^* A_0} \sigma(\nu) d\mathcal{H}^{N-1} & u \in BV(\Omega; \{a, b\}), \\ +\infty & \textit{otherwise} \end{cases}$$

where $A_0 := \{u(x) = a\}$, ν *is the outward normal to* A_0,

$$\sigma(\nu) := \lim_{T \to \infty} \inf_{u \in \mathcal{C}(TQ_\nu)} \left\{ \frac{1}{T^{N-1}} \int_{TQ_\nu} \left[W(y, u(y)) + \frac{|\nabla u(y)|^2}{2} \right] dy \right\}$$

(anisotropic surface energy)

Ansini, Braides, Chiadò Piat (2003): W homogeneous, regularization $f\left(\frac{x}{\delta(\varepsilon)}, \nabla u\right)$ ...homogenization in the regularization term leads to fundamentally different phenomena

Cell Problem

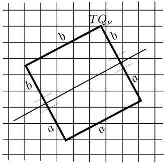
$$\sigma(\nu) = \lim_{T\to\infty} \inf_{u\in\mathcal{C}(TQ_\nu)} \left\{ \frac{1}{T^{N-1}} \int_{TQ_\nu} \left[W(y,u(y)) + \frac{|\nabla u(y)|^2}{2} \right] dy \right\}$$

where

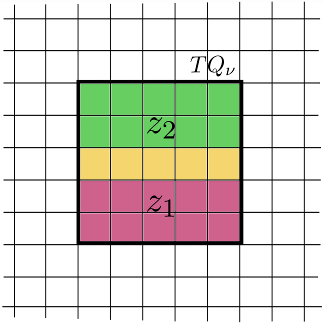
$$\mathcal{C}(TQ_\nu) := \left\{ u \in H^1(TQ_\nu;\mathbb{R}^d) : u(x) = \rho * u_{0,\nu} \text{ on } \partial(TQ_\nu) \right\}$$

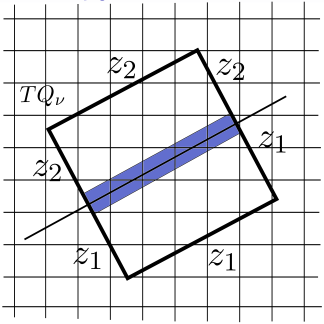
$$u_{0,\nu}(y) := \begin{cases} b & \text{if } y\cdot\nu > 0, \\ a & \text{if } y\cdot\nu < 0, \end{cases}$$

and (standard mollifier) $\rho \in C_c^\infty(\mathbb{R})$ with $\int_{\mathbb{R}} \rho = 1$



Source of Anisotropy





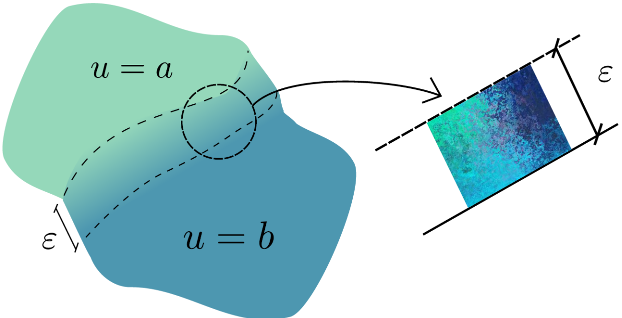
• If $\nu_A(x)$ is oriented with a direction of periodicity of W, the (local) recovery sequence would be obtained by using a rescaled version of the recovery sequence for $\sigma(\nu_A(x))$ in each yellow cube and by setting z_1 in the green region, and z_2 in the pink one.

• If $\nu_A(x)$ is not oriented with a direction of periodicity of W, the above procedure does not guarantee that we recover the desired energy, since the energy of such functions is <u>not</u> the sum of the energy of each cube.

Proof: The Road Map

- **Compactness: Bounded energy $\to BV$ structure**
- **Γ-liminf: "Lower-semicontinuity" result using blow-up techniques**
- **Γ-limsup: Recovery sequences**
  - Blow-Up Method
  - Recovery sequences for polyhedral sets with $\nu \in \mathbb{Q}^N \cap \mathbb{S}^{N-1}$
  - Density result and upper semicontinuity of σ

Challenge: Combining effects of oscillation and concentration: appearance of microstructure at scale ε within an interface of thickness ε.



Easy Case: Transition Layer Aligned with Principal Axes

If $\nu \in \{e_1, \ldots, e_N\}$, create recovery sequence by tiling optimal profiles from definition of σ.
Pick $T_k \subset \mathbb{N}$ and u_k s.t.

$$\sigma(e_N) = \lim_{k \to \infty} \frac{1}{T_k^{N-1}} \int_{T_k Q} \left[W(y, u_k(y)) + |\nabla u_k(y)|^2 \right] dy,$$

$$v_k(x) := u_k(T_k x), \text{ extended by } Q'\text{-periodicity},$$

$$v_{k,\varepsilon,r}(x) := \begin{cases} u_0(x) & |x_N| \geqslant \frac{\varepsilon T_k}{2r} \\ v_k\left(\frac{rx}{\varepsilon T_k}\right) & |x_N| < \frac{\varepsilon T_k}{2r} \end{cases}$$

$$u_{k,\varepsilon,r}(x) := v_{k,\varepsilon,r}\left(\frac{x}{r}\right) \to u \text{ in } L^1(rQ)$$

Transition Layer Aligned with Principal Axes, cont.

Blow up:

$$
\begin{aligned}
\lim_{r\to 0}\frac{F(u;rQ)}{r^{N-1}} &\leqslant \lim_{r\to 0}\lim_{\varepsilon\to 0}\frac{1}{r^{N-1}}\int_{rQ}\left[\frac{1}{\varepsilon}W(x,u_{k,\varepsilon,r})+\varepsilon|\nabla u_{k,\varepsilon,r}|^2\right]dx \\
&= \lim_{r\to 0}\lim_{\varepsilon\to 0}\int_{Q'}\int_{-\varepsilon T_k/2r}^{\varepsilon T_k/2r}\left[\frac{r}{\varepsilon}W\left(\frac{r}{\varepsilon}y, v_k\left(\frac{ry}{\varepsilon T_k}\right)\right)\right. \\
&\qquad\qquad\qquad\qquad\left. + \frac{r}{\varepsilon T_k^2}\left|\nabla v_k\left(\frac{ry}{\varepsilon T_k}\right)\right|^2\right]dy \\
&= \lim_{r\to 0}\lim_{\varepsilon\to 0}\int_{Q'}\int_{-1/2}^{1/2}\left[T_k W\left(\left(T_k\frac{rz'}{\varepsilon T_k}, T_k z_N, v_k\left(\frac{rz'}{\varepsilon T_k}, z_N\right)\right)\right.\right. \\
&\qquad\qquad\qquad\qquad\left.+\frac{1}{T_k}\left|\nabla v_k\left(\frac{rz'}{\varepsilon T_k}, z_N\right)\right|^2\right]dz
\end{aligned}
$$

Since W and v_k are **BOTH** Q'-periodic and $T_k \in \mathbb{N}$, we can use the Riemann Lebesgue Lemma:

$$\lim_{r\to 0}\lim_{\varepsilon\to 0}\int_{Q'}\int_{-1/2}^{1/2}\left[T_k W\left(\left(T_k\frac{rz'}{\varepsilon T_k}, T_k z_N\right), v_k\left(\frac{rz'}{\varepsilon T_k}, z_N\right)\right)\right.$$

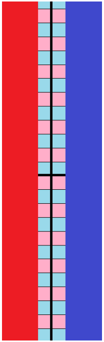
$$\left. + \frac{1}{T_k}\left|\nabla v_k\left(\frac{rz'}{\varepsilon T_k}, z_N\right)\right|^2\right]dz$$

$$= \int_{Q'}\int_{-1/2}^{1/2}\left[T_k W((T_k y', T_k z_N), v_k(y', z_N)\right.$$

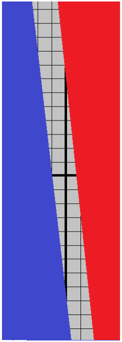
$$\left. + \frac{1}{T_k}|\nabla v_k(y', z_N)|^2 dz_N\right]dy'$$

$$= \frac{1}{T_k^{N-1}}\int_{T_k Q}\left[W(x, u_k(x)) + |\nabla u_k(x)|^2\right]dx$$

Other Transition Directions?



(a)
Aligned



(b)
Misaligned

Figure: Since W is Q-periodic, can tile along principal axes. What if the transition layer is not aligned?

Q-Periodic Implies $\lambda_\nu Q_\nu$-Periodic

Key observation: Periodic microstructure in principal directions $\rightarrow$ periodicity in other directions.

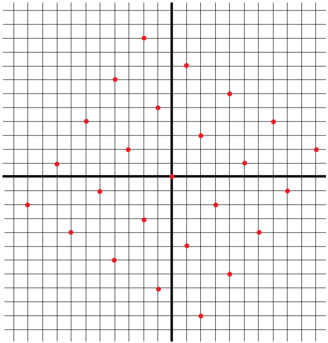


Figure: Integer lattice contains copies of itself, rotated and scaled

$\triangleright$ W is $\lambda_\nu Q_\nu$-periodic for some $\lambda_\nu \in \mathbb{N}$, and for $\nu \in \Lambda := \mathbb{Q}^N \cap \mathbb{S}^{N-1}$: Dense!

A Bit of Linear Algebra ...

Let $\nu_N \in \Lambda = \mathbb{Q}^N \cap \mathbb{S}^{N-1}$. There exist $\nu_1, \ldots, \nu_{N-1} \in \Lambda$, $\lambda_\nu \in \mathbb{N}$, s.t.

$$\nu_1, \ldots, \nu_{N-1}, \nu_N$$

o.n. basis of $\mathbb{R}^N$ and

$$W(x + n\lambda_\nu \nu_i, p) = W(x, p)$$

a.e. $x \in Q$, all $n \in \mathbb{N}$, $p \in \mathbb{R}^d$.

Also use:

$\varepsilon > 0$, $\nu \in \Lambda$, $S : \mathbb{R}^N \to \mathbb{R}^N$ rotation, $Se_N = \nu$.

Then there is a rotation $R : \mathbb{R}^N \to \mathbb{R}^N$ s.t. $Re_N = \nu$, $Re_i \in \Lambda$ all $i = 1, \ldots, N-1$, $||R - S|| < \varepsilon$

Properties of σ

- σ is well defined and finite

- the definition of σ does not depend on the choice of the mollifier

- $\sigma : \mathbb{S}^{N-1} \to [0, +\infty)$ is upper semicontinuous; actually σ is positively one-homogeneous and convex

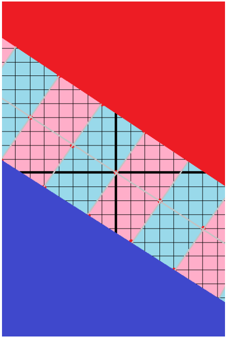
- if $\nu \in \Lambda$ then

$$\sigma(\nu) = \lim_{n\to\infty} \lim_{T\to\infty} \inf_{u \in \mathcal{C}(TQ_n)} \left\{ \frac{1}{T^{N-1}} \int_{TQ_n} \left[W(y, u(y)) + \frac{|\nabla u(y)|^2}{2} \right] dy \right\}$$

where the normals to all faces of Q_n belong to Λ

Transition Layer Aligned with $\nu \in \mathbb{Q}^N \cap \mathbb{S}^{N-1}$

Same periodic tiling technique: Use $T_k \in \lambda_\nu \mathbb{N}$.



▷ Blow up method → Recovery sequences for polyhedral sets A_0 with normals to its facets in Λ

Recovery Sequences for Arbitrary $u \in BV(\Omega; \{a, b\})$

- For $u \in BV(\Omega; \{a, b\})$, we can find $u^{(n)} \in BV(\Omega; \{a, b\})$ such that $A_0^{(n)}$ are polyhedral,

$$u^{(n)} \to u \text{ in } L^1$$

$$|Du^{(n)}|(\Omega) \to |Du|(\Omega).$$

  Since $\mathbb{Q}^N \cap \mathbb{S}^{N-1}$ dense, can require $\nu^{(n)} \in \mathbb{Q}^N \cap \mathbb{S}^{N-1}$.
- Since σ upper-semicontinuous, by Reshetnyak's,

$$\int_{\partial^* A_0} \sigma(\nu) d\mathcal{H}^{n-1} \leqslant \limsup_{n \to \infty} \int_{\partial^* A_0^{(n)}} \sigma\left(\nu^{(n)}\right) d\mathcal{H}^{n-1}$$

- Find recovery sequences $u_\varepsilon^{(n)}$ for the $u^{(n)}$ so that

$$\int_{\partial^* A_0^{(n)}} \sigma\left(\nu^{(n)}\right) d\mathcal{H}^{n-1} \leqslant \limsup_{\varepsilon \to 0^+} F_\varepsilon\left(u_\varepsilon^{(n)}\right)$$

- Diagonalize!

The Supercritical Case $\delta \ll \varepsilon$ and Fixed Wells : Riccardo Cristoferi, IF, Likhit Ganedi (2023, in arXiv)

Here

$$\frac{\varepsilon_n}{\delta_n} \to +\infty$$

In the literature (Hagerty (2019) and Ansini, Braides, Chiadò Piat (2003): $\delta \ll \varepsilon^{\frac{3}{2}}$

Recall:

$$W_{\mathrm{hom}}(z) := \min \left\{ \int_Q W^{**}(y, z + \varphi(y))\, dy \,:\, \varphi \in L^2(\Omega; \mathbb{R}^d), \int_Q \varphi \, dy = 0 \right\}$$

$$\mathcal{F}_n(u) := \int_\Omega \left[\frac{1}{\varepsilon_n} W\left(\frac{x}{\delta_n}, u(x) \right) + \varepsilon_n |\nabla u(x)|^2 \right] dx$$

Very, Very Mild Hypotheses

- W is a Carathéodory function, $W(x,\cdot)$ is Q-periodic
- $W(x,z) = 0$ iff $z \in \{a,b\}$

There exists $C > 0$ such that
- $W(x,z) \leqslant C(1+|z|^2)$ for a.e. $x \in Q$, all $z \in \mathbb{R}^d$
- $W(x,z) \geqslant \frac{1}{C}|z|^2$ for a.e. $x \in Q$, all $z \in \mathbb{R}^d$ with $|z| \geqslant C$

Remark:
- results will still hold with multiple wells and $p \geqslant 2$
- removed requirement of quadratic behavior near the wells

Theorem

$\mathcal{F}_n \xrightarrow{\Gamma} \mathcal{F}$,

$$\mathcal{F}(u) := \begin{cases} C_{\hom}\mathrm{Per}_\Omega(A_0) & u \in BV(\Omega;\{a,b\}), \\ +\infty & \textit{otherwise} \end{cases}$$

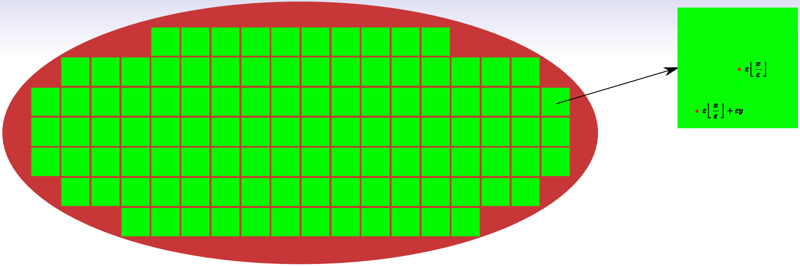
where $A_0 := \{u(x) = a\}$

$$C_{\hom} := \inf\left\{\int_1^1 2\sqrt{W_{\hom}(\gamma(t))}\,|\gamma'|\,dt\right\}$$

where γ are absolutely continuous paths with $\gamma(-1) = a$, $\gamma(1) = b$

- $\Gamma - \liminf$ Strategy: unfold only W (and throw away boundary terms)

$$\mathcal{F}_n(u) \geqslant \int_\Omega \left[\int_Q \frac{1}{\varepsilon_n} W(y, T_{\delta_n} u)\,dy + \varepsilon_n |\nabla u|^2\right] dx$$



Unfolding Operator and Two Scale Convergence

$$u_\varepsilon \overset{2-s}{\rightharpoonup} u_0 \iff T_\varepsilon(u_\varepsilon) \rightharpoonup u_0 \quad \text{in } L^p(\Omega; L^p(Q; \mathbb{R}^d))$$

Two-Scale Convergence – G.Nguetseng (1989) and Allaire (1992)

$\{u_\varepsilon\} \in L^p(\Omega; \mathbb{R}^M)$, $u_0 \in L^p(\Omega; L^p(Q; \mathbb{R}^M))$. $\{u_\varepsilon\}$ weakly two-scale converges to u_0 in $L^p(\Omega; L^p(Q; \mathbb{R}^M))$, and we write $u_\varepsilon \overset{2-s}{\rightharpoonup} u_0$, if for every $\varphi \in L^{p'}(\Omega; C_{\text{per}}(Q; \mathbb{R}^M))$

$$\lim_{\varepsilon \to 0} \int_\Omega u_\varepsilon(x) \cdot \varphi\left(x, \frac{x}{\varepsilon}\right) dx = \int_\Omega \int_Q u_0(x,y) \cdot \varphi(x,y)\, dy\, dx$$

Some Properties of the Unfolding Operator

1. $$\int_\Omega u(x)\,dx = \int_{\hat{\Omega}_\varepsilon}\int_Q T_\varepsilon(u)(x,y)\,dydx\; + \int_{\Omega\setminus\hat{\Omega}_\varepsilon} u(x)\,dx$$
2. In particular,
$$\int_\Omega W(u(x))\,dx = \int_{\hat{\Omega}_\varepsilon}\int_Q W(T_\varepsilon(u))\,dydx\; + \int_{\Omega\setminus\hat{\Omega}_\varepsilon} W(u(x))\,dx$$
3. If $u \in W^{1,p}(\Omega;\mathbb{R}^d)$, then $T_\varepsilon(\varepsilon\nabla u) = \nabla_y T_\varepsilon(u)$

• $\Gamma - \limsup$: simple. Let $\{u_n\}$ be the recovery sequence as in F-Tartar for W_{hom}

$$\begin{aligned}\limsup \mathcal{F}_n(u_n) &\leqslant \lim \int_\Omega \left[\frac{1}{\varepsilon_n} W_{\mathrm{hom}}(u_n) + \varepsilon_n |\nabla u_n|^2\right] dx \\ &+ \limsup \frac{1}{\varepsilon_n} \left| \int_\Omega \left[W\left(\frac{x}{\delta_n}, u_n(x)\right) - W_{\mathrm{hom}}(u_n(x))\right] dx \right| \\ &= C_{\mathrm{hom}} \mathrm{Per}_\Omega(\{u = a\})\end{aligned}$$

• $\Gamma - \liminf$

$$\begin{aligned}\mathcal{F}_n(u_n) &\geqslant \int_\Omega \left[\int_Q \frac{1}{\varepsilon_n} W(y, T_{\delta_n} u_n)\, dy + \varepsilon_n |\nabla u_n|^2\right] dx \\ &= \int_\Omega \left[\int_Q \frac{1}{\varepsilon_n} W(y, u_n + (T_{\delta_n} u_n - u_n))\, dy + \varepsilon_n |\nabla u_n|^2\right] dx \\ &\geqslant 2 \int_\Omega \left[\int_Q W(y, u_n + (T_{\delta_n} u_n - u_n))\, dy\right]^{\frac{1}{2}} |\nabla u_n|\, dx\end{aligned}$$

and observe that

$$||T_{\delta_n} u_n - u_n||_{L^2}(\Omega; L^2(Q; \mathbb{R}^d)) \leqslant C \frac{\delta_n}{\varepsilon_n^{1/2}}$$

and

$$||T_{\delta_n} u_n - u_n||_{L^2(\Omega; L^2(Q; \mathbb{R}^d))} ||\nabla u_n||_{L^2(\Omega; \mathbb{R}^{d\times N})} \leqslant C \frac{\delta_n}{\varepsilon_n} \to 0$$

Now "optimize" $T_{\delta_n} u_n - u_n$ (actually, need to truncate $T_{\delta_n} u_n - u_n$ appropriately, and there are boundary terms to control ... but this is the idea!): for small $\eta > 0$ choose v_n^η so that

$$\mathcal{F}_n(u_n) \geqslant 2 \int_\Omega \left[\int_Q W(y, u_n + v_n^\eta)\, dy \right]^{\frac{1}{2}} |\nabla u_n|\, dx - \eta$$

with

$$||v_n^\eta(x, \cdot)||_{L^\infty} \leqslant \eta, \quad ||v_n^\eta(x, \cdot)||_{L^2} ||\nabla_y v_n^\eta(x, \cdot)||_{L^2} \leqslant \eta$$

Then

$$\liminf \mathcal{F}_n(u_n) \geqslant \liminf 2 \int_\Omega \sqrt{W^\eta(u_n)} |\nabla u_n|\, dx - \eta$$

with

$$W^\eta(p) := \inf \left\{ \int_Q W(y, p + \psi(y))\, dy : \psi \in \mathcal{A}^\eta \right\}$$

$$\mathcal{A}^\eta = \left\{ \psi \in W_0^{1,2}(Q; \mathbb{R}^N) : ||\psi||_{L^\infty} \leqslant \eta, ||\psi||_{L^2} ||\nabla \psi||_{L^2} \leqslant 2\eta \right\}$$

Now back to the usual ($W^\eta(p) = 0$ iff $p \in \{a, b\}$, etc.)!!!

$$\begin{aligned}\liminf \mathcal{F}_n(u_n) &\geqslant \liminf 2 \int_\Omega \sqrt{W^\eta(u_n)} |\nabla u_n| \, dx - \eta \\ &\dots \\ &\geqslant C_\eta \mathrm{Per}_\Omega(\{u = a\}) - \eta\end{aligned}$$

Let $\eta \to 0$ and show that

$$C_\eta \nearrow C_{\mathrm{hom}}$$

Here use ideas of Sternberg and Zuniga for geodesics of the degenerate conformal metric

$$d_\eta(p, q) := \inf \left\{ \int_{-1}^{1} 2\sqrt{W^\eta(\gamma)} |\gamma'| \right\} dt$$

where γ are paths from p to q

The Subcritical Case $\varepsilon \ll \delta$ and Moving Wells :
Riccardo Cristoferi, IF, Likhit Ganedi (2022 to appear)

$$\mathcal{F}_\varepsilon(u) := \int_\Omega \left[\frac{1}{\varepsilon} W\left(\frac{x}{\delta(\varepsilon)}, u\right) + \frac{\varepsilon}{2}|\nabla u|^2\right] dx$$

Finite family of piecewise affine domains $\{E_i\}_{i=1}^k$ partitioning Q,

$$W(y,p) = \sum_{i=1}^{k} \chi_{E_i}(y) W_i(y,p) \quad y \in Q,\ z \in \mathbb{R}^d$$

W_i ... Lipschitz
Regime:

$$\frac{\varepsilon_n}{\delta_n} \to 0$$

$$I_n(u) := \int_\Omega \left[W\left(\frac{x}{\delta_n}, u\right) + \varepsilon_n^2 |\nabla u|^2\right] dx$$

Conditions on W

1. $$W_i(y,p) = 0 \quad \text{if and only if} \quad p \in \{a_i(y), b_i(y)\} \quad \forall y \in Q$$

   where a_i, b_i are Lipschitz
2. Behavior Near Wells: there exist $r > 0$, $C > 0$ such that
3. If $y \in Q \setminus \{a_i = b_i\}$ (**wells need NOT be separated**) then there exist $r > 0$, $R > 0$, $C > 0$ s.t.

   $$\frac{1}{C}|p - a_i(y)|^2 \leqslant W_i(y,p) \leqslant C|p - a_i(y)|^2$$

   if $y \in B(y_0, r)$ and $|p - a_i(y)| \leqslant R$, and

   $$\frac{1}{C}|p - b_i(y)|^2 \leqslant W_i(y,p) \leqslant C|p - b_i(y)|^2$$

   if $|p - b_i(y)| \leqslant R$
4. there exists $C > 0$ s. t. for all $|p| > C$, $W_i(y,p) \geqslant \frac{1}{C}|z|^2$. Furthermore, $W_i(y,p) \leqslant C(1 + |p|^2)$

Our framework includes Braides, Zeppieri (2009):

$$\int_0^1 \left[W^{(k)}\left(\frac{x}{\delta(\varepsilon)}, u\right) + \varepsilon^2 |u'|^2 \right] dx$$

Here $W : \mathbb{R} \times \mathbb{R} \to [0, \infty)$ is given by

$$W(y, s) := \begin{cases} \widetilde{W}(s - k) & y \in \left(0, \frac{1}{2}\right), \\ \widetilde{W}(s + k) & y \in \left(\frac{1}{2}, 1\right), \end{cases}$$

with $\widetilde{W}(t) := \min\{(t-1)^2, (t+1)^2\}$, and thus the wells are

$$a(y) = \begin{cases} 1 - k & \text{for } y \in \left(0, \frac{1}{2}\right), \\ 1 + k & \text{else,} \end{cases}, \quad b(y) = \begin{cases} -1 - k & \text{for } y \in \left(0, \frac{1}{2}\right). \\ -1 + k & \text{else} \end{cases}$$

Zeroth Order Result

Theorem (0^{th}-order Γ-convergence)

Let $\{u_n\} \subset W^{1,2}(\Omega;\mathbb{R}^d)$ *have bounded energy. Then (up to a subsequence, not relabeled)* $u_n \rightharpoonup u$ *in* $L^2(\Omega;\mathbb{R}^d)$ *for some* $u \in L^2(\Omega;\mathbb{R}^d)$*. Moreover,* I_n Γ*-converge to* I_0 *with respect to the weak-*L^2 *convergence:*

$$I_0(u) := \int_\Omega W_{\mathsf{hom}}(u(x))\,dx$$

$$W_{\mathsf{hom}}(z) := \min\left\{ \int_Q W^{**}(y, z+\varphi(y))\,dy \;:\; \varphi \in L^2(\Omega;\mathbb{R}^d), \int_Q \varphi\,dy = 0 \right\}.$$

Minimizers to the limit are of form:

$$u(x) = \int_Q \mu(x,y)a(y)dy + \int_Q [1-\mu(x,y)]b(y)dy$$

where $\mu \in L^2(\Omega; L^\infty(Q;[0,1]))$.

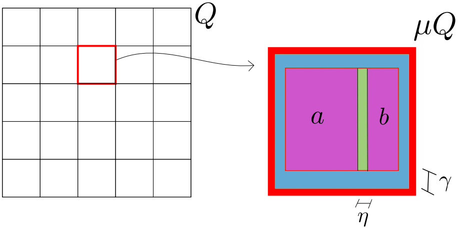
Comments on the Proof

- This was first done by Francfort and Müller (1994) for

$$\int_\Omega \left[W\left(\frac{x}{\delta}, \nabla u(x)\right) + \varepsilon^2 |\nabla^2 u(x)|^2 \right] \, dx$$

- Our proof uses simpler two-scale methods – these techniques have been applied in other contexts before, e.g. (Allaire (1992), IF and Zappale (2002))

Heuristic Scaling Analysis



$$\mathcal{F}_{\varepsilon,\delta} \sim \left[\left(\frac{\varepsilon}{\delta}\right)^2 \right] + \frac{1}{\mu}\left[\eta + \left(\frac{\varepsilon}{\delta}\right)^2 \frac{1}{\eta}\right] + \frac{1}{\mu}\left[\gamma + \left(\frac{\varepsilon}{\delta}\right)^2 \frac{1}{\gamma}\right]$$

Divide by $\frac{\varepsilon}{\delta}$:

$$\left[\frac{\varepsilon}{\delta}\right] + \frac{1}{\mu}\left[\left(\frac{\varepsilon}{\delta\eta}\right)^{-1} + \frac{\varepsilon}{\delta\eta}\right] + \frac{1}{\mu}\left[\left(\frac{\varepsilon}{\delta\gamma}\right)^{-1} + \frac{\varepsilon}{\delta\gamma}\right]$$

First Order Energy

$$\mathcal{F}_n^1(u) := \frac{\delta_n I_n(u)}{\varepsilon_n} = \int_\Omega \left[\frac{\delta_n}{\varepsilon_n} W\left(\frac{x}{\delta_n}, u(x)\right) + \varepsilon_n \delta_n |\nabla u(x)|^2 \right] dx$$

Unfolded (up to small boundary terms):

$$\mathcal{F}_n^1(u) :\approx \int_\Omega \int_Q \left[\frac{\delta_n}{\varepsilon_n} W\left(y, T_{\delta_n}(u)\right) + \frac{\varepsilon_n}{\delta_n} |\nabla_y T_{\delta_n}(u)|^2 \right] dy\, dx$$

Unfolding Operator – Cioranescu, Damlamian, Griso (2002), Visintin (2004)

$u \in L^p(\Omega; \mathbb{R}^d)$, $\varepsilon > 0$, $\hat{\Omega}_\varepsilon :=$ int $\left(\bigcup_{k' \in \mathbb{Z}^n} \{\varepsilon(Q + k') : \varepsilon(Q+k') \subset \Omega\}\right)$.
The unfolding operator $T_\varepsilon : L^p(\Omega; \mathbb{R}^d) \to L^p(\Omega; L^p(Q; \mathbb{R}^d))$ is defined as:

$$T_\varepsilon(u)(x,y) := u\left(\varepsilon \left\lfloor \frac{x}{\varepsilon} \right\rfloor + \varepsilon y\right) \quad \text{for a.e. } x \in \hat{\Omega}_\varepsilon \text{ and } y \in Q,$$

where $\lfloor \cdot \rfloor$ denotes the least integer part, and $T_\varepsilon(u)$ is extended by some $f : Q \to \mathbb{R}^d$ on $(\Omega \setminus \hat{\Omega}_\varepsilon) \times Q$.

Geodesic Energy

Define the function $\chi : \mathbb{R}^d \to \{1, \ldots, k\}$ by $\chi(y) \coloneqq i$ if $y \in E_i$

Definition

For $p, q, z_0 \in \mathbb{R}^d$ consider the class

$$\mathcal{A}(p,q,z_0) \coloneqq \left\{\gamma \in W^{1,1}((-1,1);\mathbb{R}^d) : \gamma(-1) = p, \gamma(0) = z_0, \gamma(1) = q\right\}.$$

Define $\mathrm{d_W} : \left[\, J_\chi \cup \left(\overline{Q} \setminus S_\chi\right) \,\right] \times \mathbb{R}^d \times \mathbb{R}^d \to [0, \infty)$ as

$$\mathrm{d_W}(y,p,q) \coloneqq \inf \left\{ \int_{-1}^{0} 2\sqrt{W_i(y,\gamma(t))}|\gamma'(t)|dt + \int_{0}^{1} 2\sqrt{W_j(y,\gamma(t))}|\gamma'(t)|dt \right\}$$

if $\chi^-(y) = i$ and $\chi^+(y) = j$, where the infimum is taken over points $z_0 \in \mathbb{R}^d$, and over curves $\gamma \in \mathcal{A}(p,q,z_0)$.

First Order Energy

Theorem (R. Cristoferi, IF, L. Ganedi (2021, 2022))

$\mathcal{F}_n^1(u)$ two-scale Γ-converge (Cherdantsev and Cherednichenko (2012)) with respect to the strong $L^1(\Omega; L^1(Q;\mathbb{R}^d))$ topology to the functional

$$\mathcal{F}^1(u) := \begin{cases} \displaystyle\int_\Omega \widetilde{\mathcal{F}^1}(\widetilde{u}(x,\cdot))\,dx & \text{if } u \in \mathcal{R}, \\ +\infty & \text{else,} \end{cases}$$

where

$$\widetilde{\mathcal{F}^1}(v) := \int_{\widetilde{Q}\cap J_v} \mathrm{d_W}(y, v^-(y), v^+(y))\, d\mathcal{H}^{N-1}(y).$$

where

$$\widetilde{\mathcal{R}} := \left\{ v \in L^1(\mathbb{R}^N;\mathbb{R}^d) : v \text{ is } Q\text{-periodic}, v(y) \in \{a(y), b(y)\} \text{a.e.}, \mathrm{BV}_{\mathrm{loc}}(Q_0;\mathbb{R}^d) \right\}$$

$$Q_0 := Q \setminus \{x \in Q : a(x) = b(x)\}$$

and

$$\mathcal{R} := \left\{ v \in L^2(\Omega; L^1(Q;\mathbb{R}^d)) \ : \ \widetilde{v}(x,\cdot) \in \widetilde{\mathcal{R}} \text{ for a.e. } x \in \Omega \right\},$$

where $\widetilde{v} : \mathbb{R}^N \to \mathbb{R}^d$ denotes the Q-periodic extension of $v \in L^1(Q;\mathbb{R}^d)$

Remember Lipid Rafts ...

At first order we see a local phase separation (namely in the second variable), but not a macroscopic phase separation, since this is averaged over the entire domain.

At the next order of the Γ-expansion we expect to see a macroscopic phase separation of a similar form as the one arising from homogenization of interfaces.

However, this problem will be more challenging as

$$\min \mathcal{F}^1 \text{ can be nonzero}$$

and the structure of minimizers of the mass constrained minimization problem (which is what is most interesting for applications) might be hard to identify.

Indeed:

$$\min\{\mathcal{F}^1(u) : u \in \mathcal{R}\} = 0$$

iff the Q-periodic extensions of a and b are continuous

Technical Challenges

1. Presence of two-scale variables
2. Discontinuities of the wells
3. Extension of sharp interface result of Cristoferi-Gravina (2021) **without homogenization** – Comes down to a question of uniformly bounding geodesic lengths, while in Cristoferi-Gravina (2021) the assume the condition that $W(x,p) = |p - a(x)|^2$ near the well $a(x)$ (similarly for $b(x)$), so that the geodesic is just a line
4. We do not impose wells being well-separated, they can merge (as opposed to Cristoferi-Gravina (2021))
5. Limsup inequality requires an approximation by simple functions quite delicate due to possible discontinuities in the wells

And what are we studying now?

Next order in $\Gamma-$expansion for the $\varepsilon \ll \delta$ case with fixed wells – homogenization of periodic interfacial energies

In progress with R. Cristoferi and L. Ganedi

This brings us to
• Caffarelli and de la Llave, starting in *CPAM* (2001), survey by Caffarelli in 2013
• Dirr, Lucia and Novaga (2006)
• Chambolle and Thouroude (2009)
• ETC ...

...and the search for "plane-like" minimizers ...
Oh! ...and it is the same as first $\varepsilon \to 0$ then $\delta \to 0$, so no coupling/competing effects ...

Open Problems

$$\mathcal{F}_{\varepsilon,\delta}(u) := \int_\Omega \left[\frac{1}{\varepsilon} W\left(\frac{x}{\delta}, u(x)\right) + \varepsilon |\nabla u(x)|^2 \right] dx$$

- ε . . . width of the transition layer . . . "energy" to form a phase transition
- δ . . . scale of periodicity

1. $\delta \ll \varepsilon$ and $\delta \sim \varepsilon$ with moving wells
2. . . . and stochastic homogenization! (see also, Bach, Esposito, Marziani, Zeppieri (2022), generalization of the Ambrosio-Tortorelli functional with stochastic homogenization, etc.)
3. Gradient flow: homogenization of Allen-Cahn in the subcritical and supercritical regimes. In the critical regime: R. Choksi, I. F., J. Lin, R. Venkatraman and P. Morfe, both in *Calc. Var. Partial Differential Equations* (2022)
4. **ETC! . . .**

A good place to stop . . .