Phase Separation in Heterogeneous Media

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Overview

- Brief Introduction to Cahn-Hilliard
- Phase Transitions of Heterogeneous Media, The Critical Case $\varepsilon \sim \delta$ – Riccardo Cristoferi, IF, Adrian Hagerty, and Cristina Popovici (2019, 2020)
- Phase Transitions of Heterogeneous Media, The Subcritical Case $\varepsilon \ll \delta$ and Moving Wells – Riccardo Cristoferi, IF, Likhit Ganedi (2022, in progress)
- **May not cover:** Allen-Cahn Phase Transitions of Heterogeneous Media, The Critical Case – Rustum Choksi, IF, Jessica Lin, Raghavendra Venkatraman(2021-2022, in progress)
- What is next, and open problems . . .

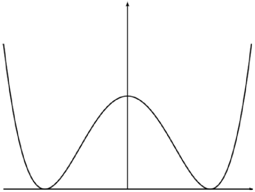
Brief Introduction to Cahn-Hilliard

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

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

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

$\mathcal{F}_\varepsilon$ 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*

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

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

A non-exhaustive list of references:

- Modica (1987)
- Sternberg (1988)
- 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

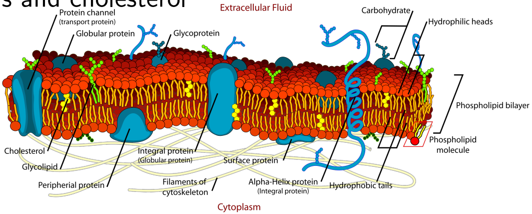


Figure: Cell Membrane– (Source: Wikipedia)

Lipid Rafts

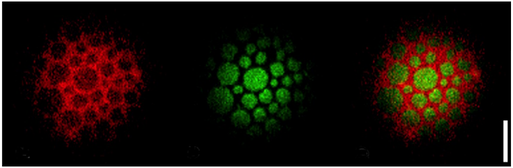


Figure: Fluorescent Imaging of Micron-scale fluid-fluid phase separation in giant unilamellar vesicles– Sengu

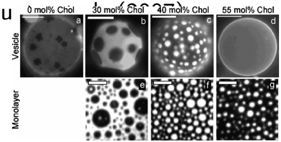


Figure: Macroscopic phase separation in a model membrane seeming to transition to a homogeneous material – Veatch and Keller (2002)

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 $\delta(\varepsilon) = \varepsilon$: 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 $\mathcal{F}_\varepsilon \xrightarrow{\Gamma} \mathcal{F}$,

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

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

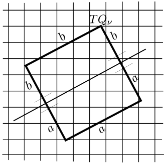
$$\sigma(\nu) = \lim_{T\to\infty} \inf_{u\in\mathcal{C}(TQ_\nu)} \left\{ \frac{1}{T^{N-1}} \int_{TQ_\nu} \left[W(y,u(y)) + \frac{|\nabla u(y)|^2}{2} \right] dy \right\}$$

where

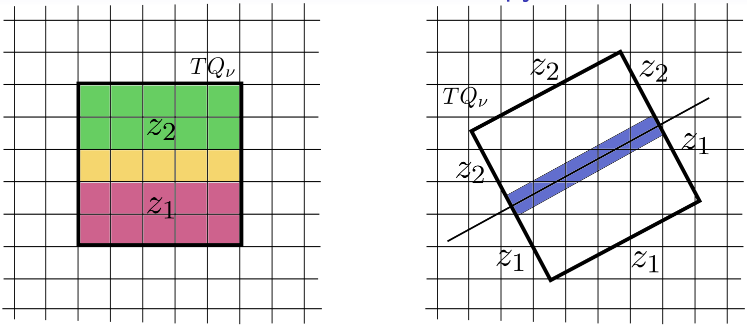
$$\mathcal{C}(TQ_\nu) := \left\{ u \in H^1(TQ_\nu;\mathbb{R}^d) : u(x) = \rho * u_{0,\nu} \text{ on } \partial(TQ_\nu) \right\}$$

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

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



Source of Anisotropy



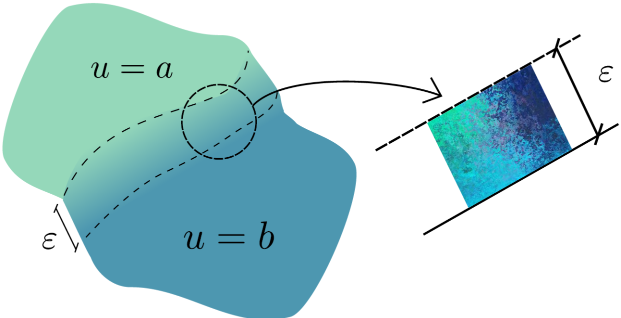
• If $\nu_A(x)$ is oriented with a direction of periodicity of W, the (local) recovery sequence would be obtained by using a rescaled version of the recovery sequence for $\sigma(\nu_A(x))$ in each yellow cube and by setting z_1 in the green region, and z_2 in the pink one.

• 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.

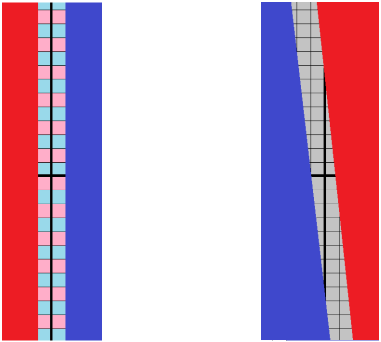
Proof: The Road Map

- **Compactness: Bounded energy $\rightarrow BV$ 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. 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.

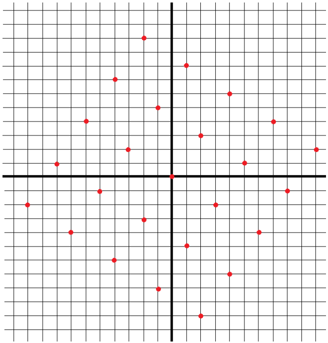


Figure: Integer lattice contains copies of itself, rotated and scaled

$\triangleright$ 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!

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

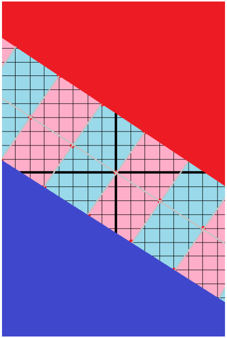
- if $\nu \in \Lambda$ then

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

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 $T_k \in \lambda_\nu \mathbb{N}$.



$\triangleright$ Blow up method $\rightarrow$ 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!

Phase Transitions of Heterogeneous Media, The Subcritical Case $\varepsilon \ll \delta$ and Moving Wells – Riccardo Cristoferi, IF, Likhit Ganedi (2022, in progress)

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

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
For general $x \in \Omega$, define $W(x,\cdot)$ by Q-periodicity
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, $W_i(y,p) \leqslant C(1 + |p|^2)$

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

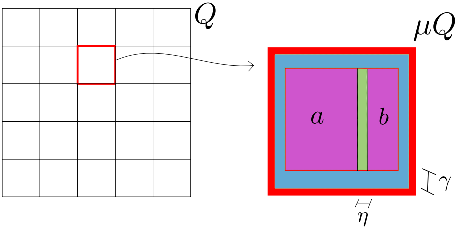
Comments on the Proof

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

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

- 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

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

Unfolded(up to small boundary terms):

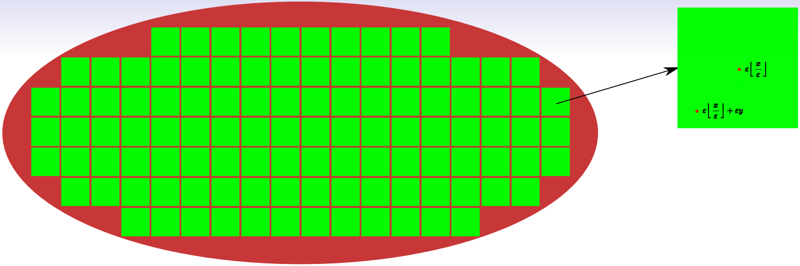
$$\mathcal{F}_n^1(u) :\approx \int_\Omega \int_Q \left[\frac{\delta_n}{\varepsilon_n} W\left(y, T_{\delta_n}(u)\right) + \frac{\varepsilon_n}{\delta_n} |\nabla_y T_{\delta_n}(u)|^2 \right] dy\, dx$$

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 $(\Omega \setminus \hat{\Omega}_\varepsilon) \times Q$.



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 $\varphi \in L^{p'}(\Omega; C_{\text{per}}(Q; \mathbb{R}^M))$

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

Geodesic Energy

Define the function $\chi : \mathbb{R}^d \to \{1, \dots, k\}$ 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

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

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))

$\mathcal{F}^1_n(u)$ 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

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

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

Allen-Cahn Phase Transitions of Heterogeneous Media, Critical Case– Rustum Choksi, IF, Jessica Lin, Raghavendra Venkatraman(2021-2022, in progress)

And now the Gradient Flow $\varepsilon \to 0^+$ asymptotics of solutions $\{u_\varepsilon\}_{\varepsilon>0}$ to a bistable reaction-diffusion PDE

$$\begin{cases} \partial_t u_\varepsilon - \Delta u_\varepsilon = -\frac{1}{\varepsilon^2} a\left(\frac{x}{\varepsilon}\right) W'(u_\varepsilon) & \text{in } \Omega_T \\ u_\varepsilon(x,0) \approx \chi_E - \chi_{\overline{E}^c} & \text{in } \Omega, \\ \frac{\partial u_\varepsilon}{\partial n} = 0 & \text{on } \partial\Omega \times (0,T], \end{cases}$$

- $\Omega \subseteq \mathbb{R}^N$, $N \geqslant 2$, smooth, bounded domain, $\Omega_T := \Omega \times (0,T]$
- $d = 1$ (scalar case), $W(x,u) := a(x)W(u)$, $W(u) := (1-u^2)^2$, double-well potential with wells at 1 and -1
- $a : \mathbb{R}^N \to \mathbb{R}$ is $\mathbb{T}^N$ periodic and C^2
- There exist $0 < \theta < \Theta < \infty$ such that $a(\cdot)$ takes values on $[\theta, \Theta]$
- $E \subseteq \mathbb{R}^N$, where ∂E is the interface between the phases 1 and -1; $u_\varepsilon(x,0) \approx \pm 1$

The heterogeneous Allen-Cahn equation is the L^2- gradient flow of $\frac{1}{\varepsilon}\mathcal{F}_\varepsilon$

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

A Familiar Asymptotic, Homogeneous Model: $a \equiv 1$

The asymptotic behaviour of (with $a \equiv 1$)

$$\partial_t u_\varepsilon - \Delta u_\varepsilon = -\frac{1}{\varepsilon^2} W'(u_\varepsilon)$$

has been studied extensively, including (but not limited to)

- Rubinstein-Sternberg-Keller (matched asymptotics)
- Classical PDE Approach: De Mottoni-Schatzman; Chen; Alikakos-Bates-Chen
- Variational Approach: Bronsard-Kohn (radial symmetry)
- Viscosity Solution Approach: Evans-Soner-Souganidis; Barles-Souganidis; Barles-Da Lio
- Geometric Measure Theory Approach: Ilmanen; Mugnai and Röger; Röger-Schätzle, Sato, Tonegawa

In all cases, it is shown that u_ε converge to solutions of some notion of generalized mean curvature flow: normal velocity = mean curvature

Characterizing the Limiting Behaviour

Homogenization Dream: Identify a function u such that $u_\varepsilon \to u$ (in some norm), where u solves an explicit "effective" PDE (a homogeneous version of the heterogeneous equation)

For

$$\partial_t u_\varepsilon - \Delta u_\varepsilon = -\frac{1}{\varepsilon^2} a\left(\frac{x}{\varepsilon}\right) W'(u_\varepsilon),$$

one expects that as $\varepsilon \to 0$, $\{u_\varepsilon\}$ converges to the (stable) equilibria ($\lim_{\varepsilon\to 0} u_\varepsilon = \pm 1$). Questions:

- What is the structure of the limiting/effective PDE (whose solution only takes the values of ± 1)?
- How will $a(\cdot)$ influence the limit?

The Transition Region when $a \equiv 1$

When $a \equiv 1$, an equilibrium solution solves

$$\Delta u = \frac{1}{\varepsilon^2} W'(u)$$

Blowing up at a point x on the interface with normal $\nu(x)$, and looking for a $1D$ profile $u(x) \approx q\left(\frac{x \cdot \nu}{\varepsilon}\right)$ leads to the heteroclinic solution:

$$q'' = W'(q), \qquad \lim_{z \to \pm\infty} q(z) = \pm 1$$

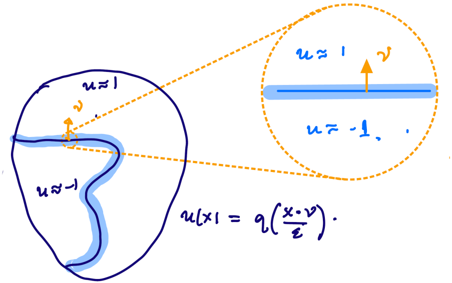


Figure: Heteroclinic connection

Equipartition of Energy

The heteroclinic ODE

$$q'' = W'(q), \qquad \lim_{z\to\infty} q(z) = \pm 1$$

is spatially invariant, so we have a conservation law, a.k.a equipartition of energy:

$$\frac{(q')^2}{2} = W(q), \qquad \lim_{z\to\infty} q(z) = \pm 1$$

With our choice of W, $q(z) = \tanh\left(\frac{z}{\sqrt{2}}\right)$
Effective surface tension:

$$\sigma = \int_{-\infty}^{\infty} \left[\frac{(q')^2}{2} + W(q)\right] dz = \int_{-\infty}^{\infty} 2\sqrt{W(q)}\frac{|q'|}{\sqrt{2}}\, dz = \sqrt{2}\int_{-1}^{1} \sqrt{W(s)}\, ds$$

What about in a periodic medium, when a is non-constant?

Eikonal Equation with Riemannian Metric

Understand "one-dimensional" solutions of the "degenerate" Eikonal equation (equipartition of energy)

$$\frac{1}{2}|\nabla u|^2 = a(y)W(u)$$

- The case $a \equiv 1$: $\frac{1}{2}|\nabla u|^2 = W(u)$ yields $u(x) = \tanh\left(\frac{x}{\sqrt{2}} \cdot \nu\right)$.
- Endow $\mathbb{R}^N$ with a Riemannian metric conformal to the Euclidean one:

$$d_{\sqrt{a}}(y_1, y_2) = \inf_{\gamma(0)=y_1, \gamma(1)=y_2} \int_0^1 \sqrt{a(\gamma(t))}|\dot{\gamma}(t)|\, dt.$$

$\Sigma_\nu := \{x : x \cdot \nu = 0\}$
$h_\nu(x) = \mathrm{sign}(x \cdot \nu) d_{\sqrt{a}}(x, \Sigma_\nu)$ ...signed distance function to the plane Σ_ν in the $\sqrt{a}-$metric. Then

$$|\nabla h_\nu(x)| = \sqrt{a}(x)$$

Recall:

$$q' = \sqrt{2W(q)} \ldots \text{with our choice of } W, q(z) = \tanh\left(\frac{z}{\sqrt{2}}\right)$$

with $q(z) \to \pm 1$ as $z \to \infty$, then $u(x) := (q \circ h_\nu)(x)$ solves (a.e.)... equipartition of energy

$$\frac{1}{2}|\nabla u|^2 = a(x)W(u).$$

When $a \equiv 1$

$$\sigma(\nu) \equiv \sigma_0 := \int_{-\infty}^{\infty} \left[W(q \circ (y \cdot \nu)) + |\nabla(q \circ (y \cdot \nu))|^2\right] d(y \cdot \nu)$$
$$= 2\int_{-1}^{1} \sqrt{W(s)}\, ds.$$

In general, would this hold with $u(x) := (q \circ h_\nu)(x)$ in place of $q \circ (y \cdot \nu)$? No, unless a is constant.

Recall:

$$\sigma(\nu) = \lim_{T\to\infty} \frac{1}{T^{N-1}} \inf\Big\{ \int_{TQ_\nu} \left[a(y)W(u) + |\nabla u|^2\right] \, dy : u \in H^1(TQ_\nu),$$
$$u = \rho * u_{0,\nu} \text{ on } \partial(TQ_\nu) \Big\}$$

$u_{0,\nu}(y) := \mathrm{sgn}(y \cdot \nu)$
Using De Giorgi's slicing method:

$$\sigma(\nu) = \lim_{T\to\infty} \frac{1}{T^{N-1}} \inf\Big\{ \int_{TQ_\nu} \left[a(y)W(u) + |\nabla u|^2\right] \, dy : u \in H^1(TQ_\nu),$$
$$u = q \circ h_\nu \text{ along } \partial(TQ_\nu) \Big\}.$$

...so

$$\sigma(\nu) \leqslant \liminf_{T\to\infty} \frac{1}{T^{N-1}} \int_{TQ_\nu} [a(y)W(q \circ h_\nu) + |\nabla(q \circ h_\nu)|^2] \, dy$$

Bounds on σ

Theorem (R. Choksi, I. F., J. Lin, R. Venkastraman (2021))

$$q(z) := \tanh(z), \quad z \in \mathbb{R}.$$

For $\nu \in \mathbb{S}^{N-1}$*, define*

$$\underline{\lambda}(\nu) := \liminf_{T\to\infty} \frac{1}{T^{N-1}} \int_{TQ_\nu} \left[a(y)W(q \circ h_\nu) + |\nabla(q \circ h_\nu)|^2\right] dy,$$

$$\overline{\lambda}(\nu) := \limsup_{T\to\infty} \frac{1}{T^{N-1}} \int_{TQ_\nu} \left[a(y)W(q \circ h_\nu) + |\nabla(q \circ h_\nu)|^2\right] dy.$$

There exist $\Lambda_0 > 0$ *and* $\lambda_0 : \mathbb{S}^{N-1} \to [0, \Lambda_0]$ *such that*

$$\overline{\lambda}(\nu) - \lambda_0(\nu) \leqslant \sigma(\nu) \leqslant \underline{\lambda}(\nu).$$

Already saw:

$$\sigma(\nu) \leqslant \underline{\lambda}(\nu).$$

Should we expect

$$\underline{\lambda}(\nu) = \sigma(\nu) = \overline{\lambda}(\nu)$$

i.e.,

$$\lambda_0(\nu) = 0?$$

No if $\nu \in \mathbb{Q}^N$: Feldman and Morfe showed that if so, then h_ν must be harmonic, and this is only if a is constant.
Also no if ν is an irrational direction.

Homogenization of the Planar Metric Problem

A natural, yet open, question concerns the large-scale homogenized behavior of h_ν, i.e., characterize the limit

$$\lim_{T\to\infty} \frac{h_\nu(Ty)}{T}, \qquad y \in \mathbb{R}^N,$$

in a suitable topology of functions. We are unable to fully resolve this question. Yet . . .

Theorem (R. Choksi, I. F. , J. Lin, R. Venkatraman (2021))

Let $\nu \in \mathbb{S}^{N-1}$, $a : \mathbb{R}^N \to \mathbb{R}$ *Bohr almost periodic, i.e.,*

$$\{a(\cdot + z) : z \in \mathbb{R}^N\}$$

is relatively compact wrt $||\cdot||_\infty$. *There exists* $c(\nu) \in [\sqrt{\theta}, \sqrt{\Theta}]$ *such that* $c(\nu) = c(-\nu)$.*, and for every sequence* $T_n \to \infty$*, and every* $K \subseteq \mathbb{R}^N$ *compact, we have*

$$\lim_{n\to\infty} \sup_{y\in K} \left| \frac{1}{T_n} h_\nu(T_n y) - c(\nu)(y\cdot\nu) \right| = 0.$$

How Can We Interpret It?

We can interpret this Theorem as a homogenization result for the Eikonal equation in half-spaces.

• Mantegazza and Mennucci (2003): for each fixed $\nu \in \mathbb{S}^{N-1}$, the functions $k_n(y) := T_n^{-1} h_\nu(T_n(y))$ and $\ell(y) := c(\nu)(y \cdot \nu)$ are the unique viscosity solutions to

$$\begin{cases} |\nabla k_n| = \sqrt{a(T_n y)} & \text{in } \{y \cdot \nu \geqslant 0\}, \\ k_n = 0 & \text{on } \Sigma_\nu, \end{cases} \quad \text{and} \quad \begin{cases} |\nabla \ell| = c(\nu) & \text{in } \{y \cdot \nu \geqslant 0\}, \\ \ell = 0 & \text{on } \Sigma_\nu. \end{cases} \tag{1}$$

Theorem $\Rightarrow$ viscosity solutions of the PDEs on the left side of (1) converge locally uniformly to the viscosity solution of the PDE on the right ("planar metric problem").

• Armstrong and Cardaliaguet (2018) introduced a viscous and stochastic version of these equations .

• Feldman and Souganidis, and Feldman (2017, 2019) studied them in the context of stochastic homogenization of geometric flows.

• We are unaware of any other homogenization results for planar metric problems in the the inviscid and periodic setting (1).

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
- $\left(\frac{\delta_n}{\varepsilon_n}\right)^2$ ... "energy" of microscopic patterns oscillating around the average of moving wells

1. Next order in $\Gamma-$expansion for this $\varepsilon \ll \delta$ case– Homogenization of interface
2. $\delta \ll \varepsilon$ expect to obtain the limit $\mathcal{F}_0^H$ of a classical Modica-Mortola functional whose potential is the homogenization of the original potential W
   - Fixed Wells

   2.1 Hagerty – our general setting, $\lim_{n\to\infty} \frac{\varepsilon_n^{3/2}}{\delta_n} = +\infty$
   2.2 With Cristoferi and Likhit, **JUST** $\lim_{n\to\infty} \frac{\varepsilon_n}{\delta_n} = +\infty$

More Open Problems

- Moving Wells

2.3 Ansini, Braides , Chiadò Piat (2003) – scalar, one dimensional case with jumping wells, and an explicit potential, $\lim_{n\to\infty} \frac{\varepsilon_n^{3/2}}{\delta_n} = +\infty$

2.4 Conjecture: will depend on $\lim_{n\to\infty} \frac{\varepsilon_n^{3/2}}{\delta_n}$

$$\frac{\varepsilon_n^{3/2}}{\delta_n} = \left[\frac{\varepsilon_n}{\left(\frac{\delta_n}{\varepsilon_n}\right)^2} \right]^{\frac{1}{2}}$$

$\lim_{n\to\infty} \frac{\varepsilon_n^{3/2}}{\delta_n} = +\infty \Rightarrow \varepsilon_n$ is dominated ($\to 0$ slower) by $\left(\frac{\delta_n}{\varepsilon_n}\right)^2$

3. Convergence of gradient flow
   - $\varepsilon \sim \delta$ with a more general well function
   - $\varepsilon \ll \delta$ open
   - $\delta \ll \varepsilon$ open
4. And then . . . stochastic homogenization.

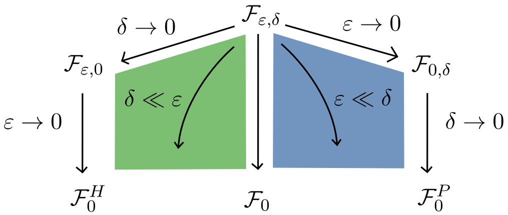


Figure: When phase transitions and homogenization act at possibly different scales

A good place to stop . . .