Cahn-Hilliard Energies: Second-Order Γ-convergence and metastable states

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Cahn–Hilliard Theory of Phase Transitions

Introduced by Van der Walls (1893), Cahn and Hilliard (1958)

$$u : \Omega \to \mathbb{R} \quad \hookrightarrow \quad \text{“phase”}$$

$$E_\varepsilon(u) := \begin{cases} \int_\Omega W(u) + \varepsilon^2 |\nabla u|^2 \, dx & \text{if } \int_\Omega u \, dx = m \\ \infty & \text{otherwise.} \end{cases}$$

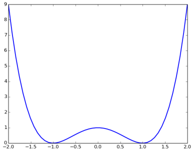

Figure: $W(u) = (u^2 - 1)^2$, a typical choice of double-well potential

Liquid-liquid (phase = density). Toy Model

Understanding the Cahn–Hilliard Energy

$$E_\varepsilon(u) := \begin{cases} \int_\Omega W(u) + \varepsilon^2 |\nabla u|^2 \, dx & \text{if } \int_\Omega u \, dx = m \\ \infty & \text{otherwise.} \end{cases}$$

The two terms dictate that

- Energetically favored phases a, b
- "Simpler" interfaces energetically favored

We note that

- $\varepsilon \hookrightarrow$ "length scale"
- u "order parameter".
- Mass Constraint $\implies$ phase transition

Goal: Understanding Limiting Behavior

$$E_\varepsilon(u) := \begin{cases} \int_\Omega W(u) + \varepsilon^2 |\nabla u|^2 \, dx & \text{if } \int_\Omega u \, dx = m \\ \infty & \text{otherwise.} \end{cases}$$

$\varepsilon \hookrightarrow$ Atomic Scale

- Static problem: Minima and minimizers
- Dyanmics: Gradient flows and metastable states

Γ-Convergence for the Cahn–Hilliard Functional

$$E_\varepsilon(u) := \begin{cases} \int_\Omega W(u) + \varepsilon^2 |\nabla u|^2 \, dx & \text{if } \int_\Omega u \, dx = m \\ \infty & \text{otherwise.} \end{cases}$$

- Fatou $\implies$ $E_\varepsilon \xrightarrow{\Gamma} E_0(u) = \int_\Omega W(u)$.
- Scaling ignores $|\nabla u|^2$
- Rescale: $F_\varepsilon := \varepsilon^{-1} E_\varepsilon = \frac{E_\varepsilon - \min E_0}{\varepsilon}$.

Properly Scaled Γ-Convergence

Modica Mortola, Gurtin, Modica, Sternberg, Kohn Sternberg, Fonseca Tartar, Baldo . . .

$F_\varepsilon \xrightarrow{\Gamma} F_0$ with

$$F_0(u) := \begin{cases} c_0 P(\{u = a\}; \Omega) & \text{if } u \in BV(\Omega; \{a, b\}), \int_\Omega u\, dx = m \\ \infty & \text{otherwise.} \end{cases}$$

The basic proof idea:

- lim inf inequality: Young's inequality, chain rule and BV lsc.
- lim sup inequality: signed distance function
- Compactness: Young's inequality, and BV compactness

Minimizers of F_0

$$F_0(u) := \begin{cases} c_0 P(\{u = a\}; \Omega) & \text{if } u \in BV(\Omega; \{a, b\}), \int_\Omega u\,dx = m \\ \infty & \text{otherwise.} \end{cases}$$

- *Partition Problem*: mass-constrained perimeter minimizers
- Minimizing sets are smooth (in dimension $n \leq 7$), are surfaces of constant mean curvature and intersect the boundary orthogonally **Gonzalez Massari Tamanini (1983), Gruter (1986)**

$$\min F_0 = c_0 \mathcal{I}_\Omega \left(\frac{b|\Omega| - m}{b - a} \right), \quad \mathcal{I}_\Omega(s) := \min\{P(E; \Omega) : |E| = s\}.$$

"Isoperimetric Function"

Higher-Order Γ-Limits

Suppose that $F_\varepsilon \xrightarrow{\Gamma} F_0$. Define

$$G_\varepsilon(u) := \frac{F_\varepsilon(u) - \min F_0}{\varepsilon}$$

Question: Does $G_\varepsilon \xrightarrow{\Gamma} \dots$?

$$\mathcal{A} := \text{ minimizers of } F_0$$

Anzellotti Baldo (1993)

Energy Asymptotics in Dimension n=1

Suppose that $u_\varepsilon \to u$ then

$$F_\varepsilon(u_\varepsilon) \geq F_0(u) + O(e^{-C_u \varepsilon^{-1}})$$

- **Carr Gurtin Slemrod (1984)**, 1 jump scaling
- **Bronsard Kohn (1990)** polynomial scaling
- **Grant (1995)**
- **Bellettini Nayam Novaga (2015)** tight bounds

Higher-Order Γ-Limit for Dimension $n > 1$

$$F_\varepsilon(u) := \begin{cases} \int_\Omega \varepsilon^{-1} W(u) + \varepsilon |\nabla u|^2 \, dx & \text{if } \int_\Omega u \, dx = m \\ \infty & \text{otherwise.} \end{cases}$$

Theorem (Dal Maso Fonseca Leoni (2014))

Suppose that $W(s) = W(-s)$ *and that* $W(s) = |s-1|^{1+\alpha}$ *near* $s = 1$, *for* $0 < \alpha < 1$. *Then if we define*

$$G_\varepsilon(u) := \begin{cases} \frac{F_\varepsilon(u) - \min F_0}{\varepsilon} & \text{if } u = 1 \text{ on } \partial\Omega \\ \infty & \text{otherwise,} \end{cases}$$

then we have that G_ε *will* Γ*-converge to* 0.

Note: Valid for anisotropic energies.

lim inf uses reduction to 1D problem.

Theorem (Pólya Szegő)

Suppose that $u \in H_0^1(\Omega)$, $u \geq 0$. Let u^* be the symmetric decreasing rearrangement of u. Then

$$\int_{\Omega^*} |\nabla u^*|^p \, dx \leq \int_{\Omega} |\nabla u|^p \, dx$$

Dirichlet Condition $u = 1$ on $\partial\Omega \implies$ Pólya Szegő

Main Results

Theorem (Leoni Murray (2015))

Suppose that $W(s) = W(-s)$ and that $W(s) = |s-1|^{1+\alpha}$ near $s = 1$, for $0 < \alpha < 1$. Furthermore suppose that $\mathcal{I}_\Omega$ is twice differentiable at $\frac{b|\Omega|-m}{b-a}$. Then if we define

$$G_\varepsilon(u) := \frac{F_\varepsilon(u) - \min F_0}{\varepsilon}$$

then we have that G_ε will Γ-converge to 0.

$$\text{Non-symmetric } W \implies G_0(u) = p(\kappa_u), \kappa_u = \text{mean curvature}$$

~~$u = 1$ on $\partial\Omega$~~

$$F_\varepsilon(u) := \begin{cases} \int_\Omega \varepsilon^{-1} W(u) + \varepsilon |\nabla u|^2 \, dx & \text{if } \int_\Omega u \, dx = m \\ \infty & \text{otherwise.} \end{cases}$$

Theorem (Leoni Murray (2015))

Suppose that $\Omega \in C^3$, with $|\Omega| = 1$ and that $W = (u^2-1)^2$. Furthermore suppose that $\mathcal{I}_\Omega$ is twice differentiable at $\frac{b|\Omega|-m}{b-a}$. Then the functional $G_\varepsilon := \frac{F_\varepsilon - \min F_0}{\varepsilon}$ satisfies

$$G_\varepsilon \xrightarrow{\Gamma} G_0(u) := \begin{cases} -\frac{(n-1)^2}{9}\kappa_u^2 & \text{if } u \in \mathcal{A} \\ \infty & \text{otherwise,} \end{cases}$$

Pólya-Szegő in bounded domains

Consider the *Isoperimetric Function* of the domain Ω:

$$\mathcal{I}_\Omega(s) := \min\{P(E;\Omega) : |E| = s\}.$$

We then define V_Ω via the differential equation

$$V_\Omega'(t) = \mathcal{I}_\Omega(V_\Omega(t)), \quad V_\Omega(0) = \frac{|\Omega|}{2},$$

and define $g_u(t) := \sup\{s : |\{u > s\}| > V_\Omega(t)\}$.

$$V_{\mathbb{R}^n}(t) = Ct^n$$

Extending the Pólya Szegő Inequality

Lemma (Leoni Murray 2015, Cianchi 1996)

For any open, connected, Lipschitz, bounded domain Ω,

$$\int |g_u'(t)|^p \mathcal{I}_\Omega(V_\Omega(t))dt \leq \int_\Omega |\nabla u|^p \, dx$$

$$\int W(g_u)\mathcal{I}_\Omega(V_\Omega(t))dt = \int_\Omega W(u)\, dx$$

- Note that $\mathcal{I}_{\mathbb{R}^n}(V_{\mathbb{R}^n}(t)) = Ct^{n-1}$.
- Equality may *not* always be attained (loss of symmetry)
- Still useful for phase transitions (esp. related to sharp interface limits)

Some remarks on proof of Main Result

$$H_\varepsilon(g_u) := \int \left(\varepsilon^{-1} W(g_u) + \varepsilon |g_u'|^2\right) \mathcal{I}_\Omega(V_\Omega(t))\, dt \leq F_\varepsilon(u)$$

- Rescale and use weak convergence
- We use a Taylor formula of order 2 on $\mathcal{I}_\Omega(V_\Omega(t))$
- Careful tail estimates use barrier methods
- $\limsup$ is straightforward

Regularity of $\mathcal{I}_\Omega$

Why should $\mathcal{I}_\Omega$ be twice differentiable?

$$\mathcal{I}_\Omega(s) := \min\{P(E;\Omega) : |E| = s\}.$$

- Ω Convex $\implies$ $\mathcal{I}_\Omega$ concave **Sternberg Zumbrun (2000)**
- For C^2 domains the function is actually semi-concave **Murray Rinaldi (2015)**

Proof Idea: Vary minimizers along normals $\hookrightarrow$ supporting hyperplanes for $\mathcal{I}_\Omega$
Assumption $\implies$ no new selection criteria ...

Competing Minimizers

Problem: Competing minimizers and rearrangement

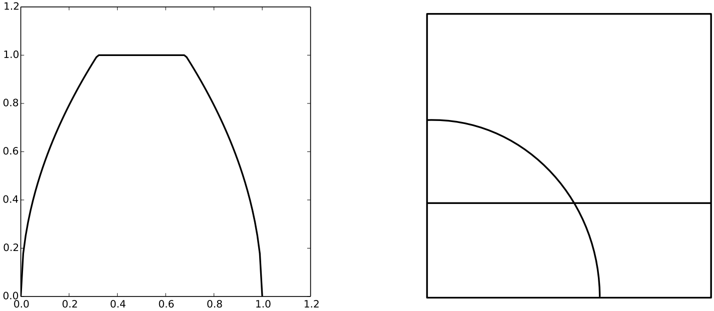

Figure: $\mathcal{I}_\Omega$ for the domain $\Omega = Q_2$, the cube in $\mathbb{R}^2$. When $\mathcal{I}_\Omega$ is not differentiable there are two competing sets minimizing the perimeter, as shown.

Localized isoperimetric functions

- $\mathcal{I}_\Omega$ does not respect "locality"
- However, converging sequence do (L^1 convergence)
- L^1 localized isoperimetric functions needed

$$\mathcal{I}_\Omega^{E_0,\delta}(t) := \inf\{P(E;\Omega) : |E| = t, \alpha(E, E_0) \leq \delta\}$$
$$\alpha(E_1, E_2) := \min\{|E_1 \backslash E_2|, |E_2 \backslash E_1|\}$$

Localized rearrangement inequalities

Proposition

If $\|u - u_0\| \leq (b-a)\delta$, $u_0 = a\chi_{E_0} + b\chi_{E_0^c}$, then the Pólya-Szegő inequality holds with $\mathcal{I}_\Omega^{E_0,\delta}(t)$ in place of $\mathcal{I}_\Omega$.

- "Local" Pólya-Szegő inequality
- Permits us to rule out competing minimizers (for liminf inequalities)

Complete Γ-limit result

Theorem (Leoni Murray (2017))

Suppose that $\Omega \in C^3$, with $|\Omega| = 1$ and that $W = (u^2-1)^2$. Then the functional $G_\varepsilon := \frac{F_\varepsilon - \min F_0}{\varepsilon}$ satisfies

$$G_\varepsilon \xrightarrow{\Gamma} G_0(u) := \begin{cases} -\frac{(n-1)^2}{9}\kappa_u^2 & \text{if } u \in \mathcal{A} \\ \infty & \text{otherwise,} \end{cases}$$

No regularity requirement on $\mathcal{I}_\Omega$.

- Utilizes "local" Pólya-Szegő inequality
- Uses non-smooth analysis ($\mathcal{I}_\Omega^{E_0,\delta}(t)$ still may be only semi-concave)

Application: Slow Motion of Gradient Flows

Gradient Flow of E_ε gives Allen–Cahn, non-local Allen–Cahn or Cahn–Hilliard

$$\partial_t u = \varepsilon^2 \Delta u - W'(u) + |\Omega|^{-1} \int_\Omega W'(u)\, dx \qquad \text{NL Allen–Cahn}$$

$$\partial_t u = -\Delta(\varepsilon^2 \Delta u - W'(u)) \qquad \text{Cahn–Hilliard}$$

Slow Dynamics Approaching Perimeter Minimizers

"Slow Manifolds" and Slow Motion

- **Fusco Hale (1989), Carr Pego (1989)** 1D interface speed $\sim e^{-K\varepsilon^{-1}}$.
- **Alikakos, Fusco, Bates, Chen, Hale, Bronsard 90's** special solutions in n-D.

More general framework: **Otto Reznikoff (2007)**

Energetic Approach ($n = 1$)

$$F_\varepsilon(u) := \begin{cases} \int_\Omega \varepsilon^{-1} W(u) + \varepsilon |\nabla u|^2 \, dx & \text{if } \int_\Omega u \, dx = m \\ \infty & \text{otherwise.} \end{cases}$$

Theorem (Bronsard Kohn (1990), (n=1), Grant (1995))

Let u_ε be a solution to the Allen-Cahn equation with $n = 1$, and fix $k > 0$. Let $u = a\chi_E + b\chi_{E^c}$ with $E \subset (-1, 1)$ a set of finite perimeter . Let $u_\varepsilon(0) \xrightarrow{L^1} u$ and let $F_\varepsilon(u_\varepsilon) \leq F_0(u) + C\varepsilon^k$. Then for any fixed $M > 0$ we have that

$$\sup_{0 \leq t \leq M\varepsilon^{-k}} \|u_\varepsilon(t) - u\|_{L^1(\Omega)} \to 0$$

Theorem (Murray Rinaldi 2016, Leoni Murray 2017)

Let $u = a\chi_E + b\chi_{E^c}$, with E a local minimizer of relative isoperimetric problem. Let $u_\varepsilon(0) \xrightarrow{L^1} u$ and let $F_\varepsilon(u_\varepsilon) \leq F_0(u) + C\varepsilon$, and let $u_\varepsilon(t)$ be a solution to the non-local Allen–Cahn Equation. Then as $\varepsilon \to 0$, for any fixed $M > 0$,

$$\sup_{0 \leq t \leq M\varepsilon^{-1}} \|u_\varepsilon(t) - u\|_{L^1(\Omega)} \to 0$$

Ansatz-Free Slow Motion in n-D, $\sim \varepsilon^{-1}$.

Possible Extensions:

- Boundary conditions?
- Extend to anisotropic energies?
- Contact energies?
- Other sharp interface problems?